E0490133 1997 281 14:54:14 REQUEST NUMBER: P281364C

JEFFREY MULLIS
US PATENT & TM OFFICE
1911 S. CLARK PLACE
CM-1, RM. 4E03, GRP. 1207
ARLINGTON, VA 22202

CA FILE PRINT FIELDS

Display

PAGE

1

CHEMICAL ABSTRACTS "CA FILE"

The CA File contains records for the documents covered in Chemical Abstracts for the time period 1967-present. Each record contains bibliographic information for the original document and indexing information, including supplementary terms (CA keywords) and CA Volume Index entries. In addition, most of the records include abstracts. Copies of most original documents may be obtained from the CAS Document Detective Service. The field codes that you may see in this offline print are listed below.

Display	
Code	Definition
AN	Accession Number
TI	Title of Document
AU	Author
IN	Patent Inventor
CS	Corporate Source
PA	Patent Assignee
S0	Source
PB	Publisher
PUI	Publisher Item Identifier
URL	Uniform Resource Locator
PI	Patent Information
D\$	Designated States (patent)
AI	Patent Application Information
PRAI	Priority Application Information
DT	Document Type
PY	Publication Year
LA	Language
IC	International Patent Classification (IPC)
ICM	Main IPC
ICS	Secondary IPC
ICA	Additional or Supplementary IPC
ICI	Index or Complementary IPC
NCL	National Patent Classification Code
cc	Classification Code (CA Section Code and Title and
	CA Section Cross-Reference Code)

CA FILE PRINT FIELDS

PAGE

2

OS Other Source
GI Graphic Image
AB Abstract

ST Supplementary Term (CA Keywords)

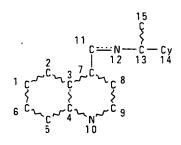
IT Index Term

Copyright © 1937 American Chemical Society (ACS)

17 ANSWERS PRINTED IN FORMAT 'BIB ABS HITSTR'

IN FILE 'CA' USING QUERY:

STR



NODE ATTRIBUTES:

NSPEC IS RC AT 15 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

220 SEA FILE=REGISTRY SSS FUL L1

17 SEA FILE=CA L2

L4 17 SEA FILE=CAPLUS L2

L5 34 SEA L2

17 DUP REM L5 (17 DUPLICATES REMOVED)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

A

L6 ANSWER 1 OF 17 CA COPYRIGHT 1997 ACS

DUPLICATE 1

AN 127:121650 CA

TI Preparation of quinoline-4-carboxamides as NK-2/NK-3 antagonists

IN Giardina, Giuseppe Arnaldo Maria; Grugni, Mario; Raveglia, Luca Francesco; Farino, Carlo

PA Smithkline Beecham S.P.A., Italy; Giardina, Giuseppe Arnaldo Maria; Grugni, Mario; Raveglia, Luca Francesco; Farino, Carlo

SO PCT Int. Appl., 61 pp. CODEN: PIXXD2

PI WO 9721680 A1 970619

DS TT, W UA, W UG, W US, W UZ, W VN, W AM, W AZ, W BY, W KG, W KZ, W MD, W RU, W TJ, W TM, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG

AI WO 96-EP5203 961122

PRAI IT 95-MI2461 951124

IT 96-MI1689 960802

DT Patent

LA English

OS MARPAT 127:121650

GI

The title compds. [I; Ar = (un)substituted aryl, C_{5-7} cycloalkadienyl (un)substituted heteroaryl; $R = C_{1-6}$ alkyl, C_{3-7} cycloalkyl, (un)substituted Ph; $R^1 = H$, C_{1-6} alkyl, aryl, etc.; $R^2 = O(CH_2)_n X$ (wherein X = (un)substituted alkyl, NH_2 , etc.), etc.; $R^3 = C_{1-6}$ alkyl, C_{3-7} cycloalkyl, (un)substituted aryl], useful for the treatment and/or prophylaxis of respiratory diseases in mammals, were prepd. Thus, reaction of $(S)-N-(\alpha-\text{ethylbenzyl})-3-\text{hydroxy-}2-\text{phenylquinoline-}4-\text{carboxamide}$ with Et bromoacetate in the presence of K_2CO_3 and KI in THF followed by hydrolysis with 37% HCl afforded (S)-I.HCl [Ar = Ph; R = Et; $R^1 = H$; $R^2 = OCH_2COOH$; $R^3 = Ph$] which showed IC_{50} of 1.9 nM

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

5

L6 ANSWER 1 OF 17 CA COPYRIGHT 1997 ACS

DUPLICATE 1

against human neurokinin-3 receptors binding in CHO cell lines.

IT ***191796-72-2P***

192704-65-7P

192704-72-6P

***192704-73-7

P***

RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of quinoline-4-carboxamides as NK-2/NK-3 antagonists)

RN 191796-72-2 CA

CN Acetic acid, [[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]-, ethyl ester, (S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192704-65-7 CA

CN Butanoic acid, 4-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]-, ethyl ester, (S)-(9CI) (CA_INDEX_NAME)

Absolute stereochemistry. Rotation (-).

RN 192704-72-6 CA

CN Benzoic acid,

2-[[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]carbonyl]-, methyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

6

RN 192704-73-7 CA

CN 2-Butenoic acid,

4-oxo-4-[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]-, methyl ester, <math>[S-(E)]-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

191796-69-7P ***191796-70-0P*** ***191796-77-7 IT ***191796-68-6P*** ***191796-80-2P*** P*** ***191796-78-8P*** ***191796-79-9P*** ***191796-81-3P*** ***191796-82-4P*** ***192704-51-1P*** ***192704-53-3 ***192704-59-9P*** ***192704-57-7P*** ***192704-55-5P*** ***192704-63-5P*** ***192704-67-9 ***192704-60-2P*** ***192704-61-3P*** ***192704-75-9P*** ***192704-77-1P*** ***192704-71-5P*** ***192704-87-3 ***192704-86-2P*** ***192704-78-2P*** ***192704-80-6P*** ***192704-92-0P*** ***192704-91-9P*** ***192704-89-5P*** ***192704-93-1P*** ***192704-95-3P*** ***192704-97-5 ***192704-94-2P*** ***192705-01-4P*** ***192705-02-5P*** ***192704-99-7P*** ***192705-04-7P*** ***192705-06-9P*** ***192705-D8-1P*** ***192816-63-0 ***192816-67-4P*** ***192816-68-5P*** ***192816-65-2P*** ***192816-69-6P*** RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of quinoline-4-carboxamides as NK-2/NK-3 antagonists) 191796-68-6 CA RN

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

7

RN 191796-68-6 CA

CN 4-Quinolinecarboxamide, 2-phenyl-3-[2-[(phenylmethyl)amino]ethoxy]-N-(1-phenylpropyl)-, monohydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

• HCI

RN 191796-69-7 CA

CN 4-Quinolinecarboxamide, $3-[2-[bis(phenylmethyl)amino]ethoxy]-2-phenyl-$\mathcal{N}-(1-phenylpropyl)-$, monohydrochloride, $(S)-(9CI)$ (CA INDEX NAME)$

Absolute stereochemistry. Rotation (-).

• HCI

RN 191796-70-0 CA

CN 4-Quinolinecarboxamide, 2-phenyl-3-[2-[(2-phenylethyl)amino]ethoxy]-N-(1-phenylpropyl)-, monohydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C RN 191796-70-0 CA

08 OCT 1997 20:02:57

PAGE

• HCI

RN 191796-77-7 CA

CN 4-Quinolinecarboxamide,

3-[2-[[[2-(hydroxymethyl)phenyl]acetyl]amino]ethoxy]-2-phenyl-\$N-(1-phenylpropyl)-, (S)- (9CI) (CAINDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-78-8 CA

CN Butanoic acid,

4-oxo-4-[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-79-9 CA

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

9

RN 191796-79-9 CA

CN 2-Butenoic acid,

4-0x0-4-[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]-, [S-(Z)]-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

RN 191796-80-2 CA

CN 4-Quinolinecarboxamide, 3-[2-[(aminoacetyl)amino]ethoxy]-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-81-3 CA

CN 4-Quinolinecarboxamide, 3-[2-[(aminophenylacetyl)amino]ethoxy]-2-phenyl-N-(1-phenylpropyl)-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

10

RN 191796-82-4 CA

RN 191796-82-4 CA

 $\textbf{CN} \qquad \textbf{4-Quinoline} carboxamide, \quad \textbf{3-[2-[(aminophenylacetyl)amino]ethoxy]-2-phenyl-} \mathcal{N}-(1-phenylpropyl)-,$

[S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192704-51-1 CA

CN Acetic acid, [[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]-, monohydrochloride,

(S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

HCI

RN 192704-53-3 CA

CN 4-Quinolinecarboxamide, 3-(2-amino-2-oxoethoxy)-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE

11

RN 192704-53-3 CA

RN 192704-55-5 CA

4-Quinolinecarboxamide, 3-[2-(dimethylamino)-2-oxoethoxy]-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) CN (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192704-57-7 CA

 $\label{lem:carbonic} \textbf{Carbonic} \ \ \textbf{acid}, \ \ \textbf{ethyl} \ \ \ \textbf{2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl} \ \ \ \textbf{ester}, \ \ \textbf{(S)-} \ \ \textbf{(9CI)}$ CN (CA INDEX NAME)

Rotation (-). Absolute stereochemistry.

192704-59-9 CA RN

4-Quinolinecarboxamide, 2-phenyl-3-[[(phenylamino)carbonyl]amino]-N-(1-phenylpropyl)-, (S)- (9CI) CN (CA INDEX NAME)

Rotation (-). Absolute stereochemistry.

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

12

RN 192704-60-2 CA

RN 192704-60-2 CA

CN Glycine, \mathcal{N} -[[[2-phenyl-4-[[[(1S)-1-phenylpropyl]amino]carbonyl]-3-quinolinyl]amino]carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192704-61-3 CA

CN 4-Quinolinecarboxamide, 3-[2-[(2,3-dihydro-1/H-inden-2-yl)amino]ethoxy]-2-phenyl-N-(1-phenylpropyl)-, monohydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

HCI

RN 192704-63-5 CA

CN 4-Quinolinecarboxamide, 3-[2-(benzoylamino)ethoxy]-2-phenyl- \mathcal{N} -(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

13

RN 192704-63-5 CA

RN 192704-67-9 CA

CN Butanoic acid, 4-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192704-71-5 CA

CN Benzoic acid,

2-[[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]carbonyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192704-75-9 CA

CN 2-Butenoic acid,

4-oxo-4-[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]-, methyl ester, <math>[S-(Z)]-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

14

RN 192704-75-9 CA

RN 192704-77-1 CA

CN 2-Butenoic acid,

 $4-oxo-4-[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy] ethyl] amino]-, \quad [S-(\mathcal{E})]-1-[[2-[[2-phenyl-4-[[3-phenylpropyl]amino]carbonyl]-3-quinolinyl]oxy] ethyl] amino]-, \quad [S-(\mathcal{E})]-1-[[3-phenylpropyl]amino]carbonyl]-3-quinolinyl]oxy] ethyl[3-phenylpropyl]amino]-, \quad [S-(\mathcal{E})]-1-[[3-phenylpropyl]amino]carbonyl]-3-quinolinyl[3-phenylpropyl]amino]-, \quad [S-(\mathcal{E})]-1-[[3-phenylpropyl]amino]carbonyl]-3-quinolinyl[3-phenylpropyl]amino]-, \quad [S-(\mathcal{E})]-1-[[3-phenylpropyl]amino]-, \quad [S-(\mathcal{E})]-1-[[3-phenylpropyl]amino]carbonyl[3-phenylpropyl]amino]-, \quad [S-(\mathcal{E})]-1-[[3-phenylpropyl]amino]carbonyl[3-phenylpropyl]amino]-, \quad [S-(\mathcal{E})]-1-[[3-phenylpropyl]amino]carbonyl[3-phenylpropyl]amino]-, \quad [S-(\mathcal{E})]-1-[[3-phenylpropyl]amino]carbonyl[3-phenylpropyl]amino]-, \quad [S-(\mathcal{E})]-1-[[3-phenylpropyl]amino]carbonyl[3-phenylpropyl]amino]carbonyl[3-phenylpropyl]amino]carbonyl[3-phenylpropyl]amino]carbonyl[3-phenylpropyl]amino]carbonyl[3-phenylpropyl]amino]carbonyl[3-phenylpropyl]amino]carbonyl[3-phenylpropylpropyl]amino]carbonyl[3-phenylpropyl$ (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

RN 192704-78-2 CA

 $4- Quinoline carboxamide, \quad 3- (cyanomethoxy)-2-phenyl- \mathcal{N}- (1-phenyl propyl)-, \quad (S)- \quad (9CI) \qquad (CA-INDEX-1)- (CA-INDEX-1)$ CN NAME)

Absolute stereochemistry. Rotation (-).

RN 192704-80-6

 $4-Quinoline carboxamide, \ 2-phenyl-3-[2-[(phenylacetyl)amino]ethoxy]-\mathcal{N}-(1-phenylpropyl)-, \ (\mathcal{S})-\ (9CI)$ CN (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

15

RN 192704-80-6 CA

Absolute stereochemistry. Rotation (-).

RN 192704-86-2 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-(1-phenylpropyl)-3-[2-[(4-pyridinylacetyl)amino]ethoxy]-, (S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192704-87-3 CA

CN 4-Quinolinecarboxamide, 2-phenyl-/V-(1-phenylpropyl)-3-[2-[(3-pyridinylacetyl)amino]ethoxy]-, (S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192704-89-5 CA

CN 4-Quinolinecarboxamide, 2-phenyl-/V-(1-phenylpropyl)-3-[2-[(2-pyridinylacetyl)amino]ethoxy]-, (S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE

16

RN 192704-89-5 CA

RN 192704-91-9 CA

CN Benzoic acid,

2-[2-oxo-2-[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]ethyl]-, (S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192704-92-0 CA

CN Benzeneacetic acid,

2-[[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]carbonyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192704-93-1 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-(1-phenylpropyl)-3-(4-pyridinylmethoxy)-, (S)- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

17

RN 192704-93-1 CA Absolute stereochemistry.

RN 192704-94-2 CA

CN 2,3-Pyrazinedicarboxamide,

N-[3-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]propyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192704-95-3 CA

CN 4-Quinolinecarboxamide, 2-phenyl- \mathcal{N} -(1-phenylpropyl)-3-[2-[(pyrazinylcarbonyl)amino]ethoxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192704-97-5 CA

CN 4-Quinolinecarboxamide, 3-[2-[[(3-aminopyrazinyl)carbonyl]amino]ethoxy]-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

18

RN 192704-97-5 CA

Absolute stereochemistry.

RN 192704-99-7 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-(1-phenylpropyl)-3-[3-[(pyrazinylcarbonyl)amino]propoxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192705-01-4 CA

CN 4-Quinolinecarboxamide,

 $3-[2-[[[2-[(methylamino)methyl]phenyl]acetyl]amino]ethoxy]-2-phenyl-\mathcal{N}-(1-phenylpropyl)-, \ \ \langle \mathcal{S}\rangle-\ \ \ \langle \mathcal{S}\rangle-\ \ \langle$

Absolute stereochemistry.

RN 192705-02-5 CA

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

19

RN 192705-02-5 CA

CN 4-Quinolinecarboxamide,

2-phenyl-N-(1-phenylpropyl)-3-[2-[[[2-(1-pyrrolidinylmethyl)phenyl]acetyl]amino]ethoxy]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192705-04-7 CA

CN 4-Quinolinecarboxamide,

 $2-phenyl-\mathcal{N}-(1-phenylpropyl)-3-[2-[[[2-[2-(1-pyrrolidinyl)ethoxy]phenyl]acetyl]amino]ethoxy]-, \ (S)- \ (9CI) \ (CA INDEX NAME)$

Absolute stereochemistry.

RN 192705-06-9 CA

CN 4-Quinolinecarboxamide, 3-[2-[[(2-hydroxyphenyl)acetyl]amino]ethoxy]-2-phenyl-/V-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

20

RN 192705-06-9 CA

RN 192705-08-1 CA

CN 4-Quinolinecarboxamide, 3-[2-[[(2-methoxyphenyl)acetyl]amino]ethoxy]-2-phenyl-<math>N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 192816-63-0 CA

CN 4-Quinolinecarboxamide,

 $3-[2-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)amino]ethoxy]-2-phenyl-$\mathcal{N}-(1-phenylpropyl)-,$ monohydrochloride, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

• HCI

RN 192816-65-2 CA

CN 4-Quinolinecarboxamide, 3-[2-[(2,3-dihydro-1*H*-inden-2-yl)amino]ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

21

RN 192816-65-2 CA

RN 192816-67-4 CA

CN 4-Quinolinecarboxamide, 2-phenyl-3-[2-[(phenylmethyl)amino]ethoxy]-/V-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192816-68-5 CA

CN 4-Quinolinecarboxamide, 3-[2-[bis(phenylmethyl)amino]ethoxy]-2-phenyl- \mathcal{N} -(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192816-69-6 CA

CN 4-Quinolinecarboxamide,

3-[2-[(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)amino]ethoxy]-2-phenyl-N-(1-phenylpropyl)-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

22

RN 192816-69-6 CA

IT ***174636-16-9P*** ***174636-32-9P***

191796-73-3P

***191796-74-4

192705-11-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of quinoline-4-carboxamides as NK-2/NK-3 antagonists)

RN 174636-16-9 CA

CN 4-Quinolinecarboxamide, 3-amino-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

RN 174636-32-9 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

RN 191796-73-3 CA

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

23

RN 191796-73-3 CA

CN 4-Quinolinecarboxamide,

3-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethoxy]-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CAINDEX NAME)

Absolute stereochemistry. Rotation (~).

RN 191796-74-4 CA

CN 4-Quinolinecarboxamide, 3-(2-aminoethoxy)-2-phenyl-/V-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 192705-11-6 CA

CN Carbamic acid,

[2-oxo-1-phenyl-2-[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy] ethyl] - gH-fluoren-9-ylmethyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Copyright © 1997 American Chemical Society (ACS)

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57 PAGE

24

Copyright © 1997 American Chemical Society (ACS)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

25

L6 ANSWER 2 OF 17 CA COPYRIGHT 1997 ACS

DUPLICATE 2

AN 127:81363 CA

TI Preparation of 4-quinolinecarboxamide salt derivatives as neurokinin-3 receptor antagonists

IN Giardina, Giuseppe Arnaldo Maria; Farina, Carlo; Grugni, Mario; Raveglia, Luca Francesco

PA Smithkline Beecham S.P.A., Italy; Giardina, Giuseppe Arnaldo Maria; Farina, Carlo; Grugni, Mario; Raveglia, Luca Francesco

SO PCT Int. Appl., 26 pp. CODEN: PIXXD2

PI WO 9719928 A1 970605

DS TT, W UA, W UG, W US, W UZ, W VN, W AM, W AZ, W BY, W KG, W KZ, W MD, W RU, W TJ, W TM, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG

AI WO 96-EP5210 961122

PRAI GB 95-24137 951124

DT Patent

LA English

OS MARPAT 127:81363

GI

The title salt compds. [I; A = (un)substituted Ph, (un)substituted naphthyl, (un)substituted C_{5-7} cycloalkadienyl, (un)substituted single or fused-ring heterocyclyl; R = C_{1-8} alkyl, cycloalkyl, (un)substituted Ph, (un)substituted 5-member heterocyclyl, etc.; R1, R2 = H, alkyl; R3, R4 = H, alkyl, alkenyl, aryl, alkoxy, OH, halogen, NO₂, CN, (un)substituted NH₂, etc.; R5 = alkyl, cycloalkyl, (un)substituted aryl, etc.; X = O, S, NC:N], useful as neurokinin-3 receptor antagonists, are prepd. Thus, $(S)-(-)-N-(\alpha-\text{ethylbenzyl})-3-\text{hydroxy-2-phenyl-4-quinolinecarboxamide}$ was dissolved in aq. MeOH contg. NaOH and heated to 40°, producing $(S)-(+)-N-(\alpha-\text{ethylbenzyl})-3-\text{hydroxy-2-phenyl-4-quinolinecarboxamide}$ sodium salt sesquihydrate, m.p. 110° (decompn.), which demonstrated a K_i of 4.8 nM for the displacement of [3H]-senktide from guinea pig cortex membrane-derived NK₃ receptors.

IT ***191786-18-2P***

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

26

L6 ANSWER 2 OF 17 CA COPYRIGHT 1997 ACS

DUPLICATE 2

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 4-quinolinecarboxamide salt derivs. as neurokinin-3 receptor antagonists)

RN 191786-18-2 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl- \mathcal{N} -(1-phenylpropyl)-, monosodium salt, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Na

IT ***174636-32-9P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

(prepn. of 4-quinolinecarboxamide salt derivs. as neurokinin-3 receptor antagonists)

RN 174636-32-9 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

Copyright © 1997 American Chemical Society (ACS)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

27

L6 ANSWER 3 OF 17 CA COPYRIGHT 1997 ACS

DUPLICATE 3

AN 127:95205 CA

TI Preparation of quinoline-derivative NK₃ receptor antagonists

IN Giardina, Giuseppe Arnaldo Maria; Farina, Carlo; Grugni, Mario; Raveglia, Luca Francesco

PA Smithkline Beecham S.P.A., Italy; Giardina, Giuseppe Arnaldo Maria; Farina, Carlo; Grugni, Mario; Raveglia, Luca Francesco

SO PCT Int. Appl., 101 pp.

CODEN: PIXXD2

PI WO 9719927 A1 970605

DS W: JP, US

RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

AI WO 96-EP5209 961122

PRAI GB 95-24104 951124

DT Patent

LA English

OS MARPAT 127:95205

GI

The title compds. [I; A = (un)substituted Ph, (un)substituted naphthyl, C_{5-7} cycloalkdienyl, (un)substituted heterocyclyl; $R = C_{1-8}$ alkyl, C_{3-7} cycloalkyl, C_{4-7} cycloalkylalkyl, (un)substituted Ph, phenylalkyl, etc.; R^1 , $R^2 = H$, C_{1-6} alkyl, or together form a $(CH_2)_n$, etc.; n = 3-5; R^3 , $R^4 = H$, C_{1-6} alkyl, C_{1-6} alkenyl, aryl, C_{1-6} alkoxy, hydroxy, halogen, nitro, cyano, carboxy, carboxamido, sulfonamido, C_{1-6} alkoxycarbony, trifluoromethyl, acyloxy, phthalimido, (un)substituted amino, etc.; $R^5 = C_{1-6}$ alkyl, C_{3-7} cycloalkyl, etc.; X = 0, S, NC:N; etc.], which are NK_3 receptor antagonists (no data), are prepd. Thus, α -methylbenzylamine was amidated with 2-phenylquinoline-4-carbonyl chloride, producing $N-(\alpha$ -methylbenzyl)-2-phenyl-4-quinolinecarboxamide, m.p. 156-157°.

IT ***174635-48-4P***

174635-49-5P

174635-50-8P

***174635-51-9

P*** ***174635-52-0P*** ***174635-55-3P*** ***17

P*** ***174635-54-2P*** ***174635-57-5P*** ***1

***174635-58-6

P***

174635-59-7P

174635-60-0P

174635-61-1P

174635-62-2P

174635-63-3P

174635-64-4P

***174635-65-5

P***

174635-66-6P

174635-68-8P

174635-69-9P

CA FILE SEARCH RESULTS - P281364C

(

08 OCT 1997 20:02:57

PAGE

28

```
ANSWER 3 OF 17 CA COPYRIGHT 1997 ACS
L6
                                                                        DUPLICATE 3
       ***174635-70-2P***
                                 ***174635-71-3P***
                                                           ***174635-72-4P***
                                                                                     ***174635-73-5
       P***
                   ***174635-74-6P***
                                             ***174635-75-7P***
                                                                       ***174635-76-8P***
       ***174635-77-9P***
                                 ***174635-78-0P***
                                                           ***174635-79-1P***
                                                                                     ***174635-80-4
                   ***174635~81-5P***
                                             ***174635-82-6P***
                                                                       ***174635-83-7P***
       ***174635-84-8P***
                                 ***174635-85-9P***
                                                           ***174635-86-0P***
                                                                                      ***174635-87-1
       P***
                   ***174635-88-2P***
                                             ***174635-89-3P***
                                                                        ***174635-90-6P***
       ***174635-91-7P***
                                 ***174635-92-8P***
                                                           ***174635-93-9P***
                                                                                     ***174635-94-0
       P***
                   ***174635-95-1P***
                                             ***174635-96-2P***
                                                                       ***174635-97-3P***
       ***174635-98-4P***
                                 ***174636-00-1P***
                                                           ***174636-01-2P***
                                                                                     ***174636-03-4
       P***
                   ***174636-04-5P***
                                             ***174636-05-6P***
                                                                       ***174636-06-7P***
       ***174636-07-8P***
                                 ***174636-09-0P***
                                                           ***174636-10-3P***
                                                                                     ***174636-11-4
                   ***174636-12-5P***
                                          ***174636-13-6P***
                                                                      ***174636-14-7P***
       ***174636-15-8P***
                                 ***174636-16-9P***
                                                          ***174636-17-0P***
                                                                                    ***174636-18-1
                   ***174636-19-2P***
                                            ***174636-20-5P***
                                                                      ***174636-21-6P***
       ***174636-22-7P***
                                 ***174636-23-8P***
                                                           ***174636-24-9P***
                                                                                      ***174636-25-0
                  ***174636-26-1P***
                                            ***174636-27-2P***
                                                                       ***174636-28-3P***
      ***174636-29-4P***
                                 ***174636-30-7P***
                                                           ***174636-31-8P***
                                                                                     ***174636-32-9
                   ***174636-33-0P***
                                             ***174636-34-1P***
                                                                       ***174636-35-2P***
       ***174636-36-3P***
                                 ***174636-37-4P***
                                                           ***174636-38-5P***
                                                                                      ***174636-39-6
                  ***174636-40-9P***
                                             ***174636-42-1P***
                                                                       ***174636-43-2P***
      ***174636-44-3P***
                                 ***174636-46-5P***
                                                           ***174636-47-6P***
                                                                                      ***174636-49-8
                  ***174636-50-1P***
                                            ***174636-51-2P***
                                                                      ***174636-52-3P***
      ***174636-53-4P***
                                 ***174636-54-5P***
                                                           ***174636-55-6P***
                                                                                     ***174636-56-7
                  ***174636-57-8P***
                                             ***174636-58-9P***
                                                                       ***174636~60-3P***
      ***174636-61-4P***
                                                          ***189815-94-9P***
                                ***174636-62-5P***
                                                                                    ***191796-73-3
                  ***191939-91-0P***
                                           ***191939-92-1P***
       RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP
      (Preparation); USES (Uses)
            (prepn. of quinoline-deriv. NK3 receptor antagonists)
RN
       174635-48-4
CN
       4-Quinolinecarboxamide, 2-phenyl-N-(1-phenylethyl)- (9CI) (CA INDEX NAME)
```

RN 174635-49-5 CA

CA FILE SEARCH RESULTS ~ P281364C

08 OCT 1997 20:02:57

PAGE

32

RN 174635-58-6 CA

RN 174635-59-7 CA

CN Benzeneacetic acid, α -[[[2-(2-furanyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-60-0 CA

CN Benzeneacetic acid, α -[[[2-(4-pyridinyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-61-1 CA

CN 2-Thiopheneacetic acid, α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

33

RN 174635-61-1 CA

RN 174635-62-2 CA

CN Benzenepropanoic acid, β -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) INDEX NAME)

RN 174635-63-3 CA

CN 1,4-Cyclohexadiene-1-acetic acid, α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 174635-64-4 CA

CN 4-Quinolinecarboxamide, N-(2-hydroxy-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE

34

RN 174635-64-4 CA

RN 174635-65-5 CA

CN 4-Quinolinecarboxamide, 3-methoxy-2-phenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

174635-66-6 RN CA

CN 4-Quinolinecarboxamide, 3-butyl-2-phenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

174635-68-8 RN CA

4-Quinolinecarboxamide, 3-hexyl-2-phenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME) CN

174635-69-9 RN CA

4-Quinolinecarboxamide, 3-methyl-2-phenyl-/V-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) CN Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

35

RN 174635-69-9 CA

RN 174635-70-2

CN 4-Quinolinecarboxamide, 3-methyl-2-phenyl-N-(1-phenylpropyl)-, (R)- (9CI) (CA INDEX NAME) Rotation (+). Absolute stereochemistry.

RN 174635-71-3 CA

CN Benzeneacetic acid, α -[[[2-(2-methoxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-72-4 CA

CN 4-Quinolinecarboxamide, 2,3-diphenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

36

RN 174635-72-4 CA

RN 174635-73-5 CA

Benzeneacetic acid, α -[[[2-(2-fluorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA CN INDEX NAME)

RN 174635-74-6

CN 4-Quinolinecarboxamide, N-[1-(3,4-dichlorophenyl)propyl]-2-phenyl- (9CI) (CA INDEX NAME)

RN 174635-75-7 CA

4-Quinolinecarboxamide, N-(2-hydroxy-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME) CN

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

37

RN 174635-75-7 CA

RN 174635-76-8 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 174635-77-9 CA

CN Benzeneacetic acid, α -[[(3-methyl-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-78-0 CA

CN 4-Quinolinecarboxamide, 3-methyl-2-phenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 174635-79-1 CA

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

38

RN 174635-79-1 CA

CN Benzeneacetic acid, α -[[(7-chloro-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-80-4 CA

CN Benzeneacetic acid, α -[[(6-methyl-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-81-5 CA

CN 4-Quinolinecarboxamide, N-(2-methoxy-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 174635-82-6 CA

CN Benzeneacetic acid, α -[[(6-chloro-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE

39

CA RN 174635-82-6

RN 174635-83-7 ĊΑ

Benzeneacetic acid, α -[[(3-ethyl-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) CN INDEX NAME)

RN 174635-84-8 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-(1-phenylbutyl)- (9CI) (CA INDEX NAME)

RN 174635-85-9 CA

CN 4-Quinolinecarboxamide, 3-ethyl-2-phenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 174635-86-0

CN $4-Quinoline carboxamide, \quad 3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-2-phenyl-\mathcal{N}-(1-phenylpropyl)- \quad (9CI)$ (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

40

RN 174635-86-0 CA

RN 174635-87-1 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-(1-phenylpropyl)-3-propyl- (9CI) (CA INDEX NAME)

RN 174635-88-2 CA

CN 4-Quinolinecarboxamide, 6-bromo-2-(4-bromophenyl)-3-methyl- \mathcal{N} -(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 174635-89-3 CA

CN 4-Quinolinecarboxamide, 6-bromo-3-methyl-2-phenyl- \mathcal{N} -(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

41

RN 174635-89-3 CA

RN 174635-90-6 CA

CN Benzeneacetic acid, α -[[(6-methoxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-91-7 CA

Benzeneacetic acid, α -[[[2-(2-benzofuranyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) CN (CA INDEX NAME)

RN 174635-92-8 CA

CN 4-Quinolinecarboxamide, N-(1,2-diphenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE

42

RN 174635-93-9 CA

RN 174635-93-9 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-(2,2,2-trifluoro-1-phenylethyl)- (9CI) (CA INDEX NAME)

RN 174635-94-0 CA

CN 4-Quinolinecarboxamide, 3-methoxy-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

RN 174635-95-1 CA

CN 4-Quinolinecarboxamide, 3-ethyl-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

RN 174635-96-2 CA

CN 4-Quinolinecarboxamide, N-[1-(4-chlorophenyl)propyl]-2-phenyl- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C RN

08 OCT 1997 20:02:57

PAGE

43

174635-96-2 CA

RN 174635-97-3 CA

CN Benzeneacetic acid, α -[methyl[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-98-4

CN Benzeneacetic acid, α -[[[2-(3-thienyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) INDEX NAME)

RN 174636-00-1 CA

Benzeneacetic acid, α -[[[2-(1H-pyrrol-2-yl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) CN (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C RN

08 OCT 1997 20:02:57

PAGE

44

174636-00-1 CA

RN 174636-01-2 CA

Benzeneacetic acid, α -[[[2-(2-thiazolyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) CN INDEX NAME)

RN 174636-03-4 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-(1-phenylpentyl)- (9CI) (CA INDEX NAME)

CA RN 174636-04-5

CN Benzeneacetic acid, α -[[[2-(4-methylphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

45

RN 174636-05-6 CA

RN 174636-05-6 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-(1-phenyloctyl)- (9CI) (CA INDEX NAME)

RN 174636-06-7 CA

CN Benzeneacetic acid, $\alpha = ([2-(2-methylphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)$

RN 174636-07-8 CA

CN Benzeneacetic acid, α -[[[2-(4-methoxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-09-0 CA

CN Benzeneacetic acid, α -[[[2-(4-hydroxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57-

CA

PAGE

46

RN 174636-09-0 CA

RN 174636-10-3

Benzeneacetic acid, α -[[[2-(1,3-benzodioxol-5-yl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) CN (CA INDEX NAME)

174636-11-4 RN

4-Quinolinecarboxamide, N-(1-methyl-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME) CN

174636-12-5 RN CA

CN 4-Quinolinecarboxamide, N-[1-(4-methylphenyl)propyl]-2-phenyl- (9CI) (CA INDEX NAME)

47

RN 174636-13-6 CA

CN Benzeneacetic acid, α -[[[2-(1H-pyrrol-3-yl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-14-7 CA

CN Benzeneacetic acid, α -[[[2-(3,4-dichlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-15-8 CA

CN 4-Quinolinecarboxamide, N-(2-amino-1-phenylethyl)-2-phenyl-, (R)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

RN 174636-16-9 CA

CN 4-Quinolinecarboxamide, 3-amino-2-phenyl- \mathcal{N} -(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

RN 174636-17-0 CA

CN 4-Quinolinecarboxamide, 3-chloro-2-phenyl- \wedge -(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

RN 174636-18-1 CA

CN 4-Quinolinecarboxamide, 3-bromo-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

49

RN 174636-18-1 CA

RN 174636-19-2 CA

CN 4-Quinolinecarboxamide, N-(2-methyl-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 174636-20-5 CA

CN 4-Quinolinecarboxamide, 2-phenyl- \mathcal{N} -(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

RN 174636-21-6 CA

CN 4-Quinolinecarboxamide, 2-phenyl- \mathcal{N} -(1-phenylpropyl)-, (\mathcal{R})- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (+).

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

50

RN 174636-22-7 CA RN 174636-22-7 CA

CN Benzeneacetic acid, α -[[(6-fluoro-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA

INDEX NAME)

RN 174636-23-8 CA

CN Benzeneacetic acid, α -[[(2-cyclohexyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-24-9 CA

CN Benzeneacetic acid, α -[[[2-(3-chlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-25-0 CA

CN Benzeneacetic acid, α -[[[2-(2-chlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

51

RN 174636-26-1 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 174636-27-2 CA

CN Benzeneacetic acid, α -[[[8-(acetyloxy)-2-phenyl-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-28-3 CA

CN Benzeneacetic acid, α -[[(8-hydroxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE

52

RN 174636-28-3 CA

RN 174636-29-4 CA

Benzeneacetic acid, α -[[[2-(2,4-dichlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) CN (CA INDEX NAME)

174636-30-7 CA RN

Benzeneacetic acid, 4-hydroxy- α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, CN monohydrochloride, (R)- (9CI) (CA. INDEX NAME)

Absolute stereochemistry. Rotation (-).

• HCI

174636-31-8 RN CA

CN 4-Quinolinecarboxamide, N-(diphenylmethyl)-2-phenyl- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

53

RN 174636-32-9 CA

RN 174636-32-9 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

RN 174636-33-0 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl- \mathcal{N} -(1-phenylpropyl)-, (\mathcal{R})- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (+).

RN 174636-34-1 CA

CN Benzeneacetic acid, α -[[(3-hydroxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 174636-35-2 CA

CN 4-Quinolinecarboxamide, N-[2-(dimethylamino)-1-phenylethyl]-2-phenyl-, (R)- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

54

RN 174636-35-2 CA

Absolute stereochemistry. Rotation (-).

RN 174636-36-3 CA

CN 4-Quinolinecarboxamide, \mathcal{N} -[2-(dimethylamino)-2-oxo-1-phenylethyl]-2-phenyl- (9CI) (CA INDEX NAME)

RN 174636-37-4 CA

CN 4-Quinolinecarboxamide, N-(2-amino-2-oxo-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 174636-38-5 CA

CN 4-Quinolinecarboxamide, N-[2-oxo-1-phenyl-2-(1-pyrrolidinyl)ethyl]-2-phenyl- (9CI) (CA INDEX NAME)

PAGE

55

RN 174636-38-5 CA

RN 174636-39-6 CA

Benzeneacetic acid, α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, monohydrochloride, (R)- (9CI) CN (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

• HCI

RN 174636-40-9 CA

Benzeneacetic acid, α -[[[2-(4-chlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA CN INDEX NAME)

RN 174636-42-1 CA

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

56

RN 174636-42-1 CA

CN Benzeneacetic acid, α -methyl- α -[methyl[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

• HCI

RN 174636-43-2 CA

CN 4-Quinolinecarboxamide, N-(2-oxo-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 174636-44-3 CA

CN 4-Quinolinecarboxamide, N-(3-hydroxy-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

RN 174636-46-5 CA

CN 4-Quinolinecarboxamide, 3-(acetylamino)-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

57

RN 174636-46-5 CA

RN 174636-47-6 CA

CN 4-Quinolinecarboxamide, 3-[3-(dimethylamino)propoxy]-2-phenyl-/V-(1-phenylpropyl)-,

monohydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

• HCI

RN 174636-49-8 CA

CN 4-Quinolinecarboxamide, 3-(2-aminoethoxy)-2-phenyl-N-(1-phenylpropyl)-, monohydrochloride, (S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

58

RN 174636-50-1 CA

RN 174636-50-1 CA

 $\textbf{CN} \qquad \textbf{4-Quinoline} \\ \textbf{a-phenyl-} \mathcal{N}-(\textbf{1-phenylpropyl})-\textbf{3-[2-(1-pyrrolidinyl)ethoxy]-,} \\ \text{monohydrochloride,}$

(S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

• HCI

RN 174636-51-2 CA

CN 4-Quinolinecarboxamide, 3-[[(dimethylamino)acetyl]amino]-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 174636-52-3 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-N-(1-methyl-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 174636-53-4 CA

CN 4-Quinolinecarboxamide, 3-amino-N-(1-methyl-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE

59

RN 174636-53-4 ÇA

RN 174636-54-5 CA

4-Quinolinecarboxamide, 5-methyl-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) CN Absolute stereochemistry. Rotation (-).

174636-55-6 CA RN

CN 4-Quinolinecarboxamide, N-(2-hydroxy-1-phenylpropyl)-3-methyl-2-phenyl- (9CI) (CA INDEX NAME)

RN 174636-56-7 CA

4-Quinolinecarboxamide, 3-methyl-/V-(2-oxo-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME) CN

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

60

RN 174636-57-8 CA

RN 174636-57-8 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-[1-(4-pyridinyl)propyl]- (9CI) (CA INDEX NAME)

RN 174636-58-9 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-[1-(2-thienyl)propyl]- (9CI) (CA INDEX NAME)

RN 174636-60-3 CA

CN 4-Quinolinecarboxamide, 7-methoxy-3-methyl-2-phenyl-/\(\mathcal{N}\)-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

61

RN 174636-61-4 CA

RN 174636-61-4 CA

CN 4-Quinolinecarboxamide, 3-amino-5-methyl-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174636-62-5 CA

CN 4-Quinolinecarboxamide, 3-methoxy-5-methyl-2-phenyl- \mathcal{N} -(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 189815-94-9 CA

CN Benzeneacetic acid, 4-methoxy- α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

62

RN 189815-94-9 CA

RN 191796-73-3 CA

CN 4-Quinolinecarboxamide,

3-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethoxy]-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191939-91-0 CA

CN 4-Quinolinecarboxamide, 3-[2-(dimethylamino)ethoxy]-2-phenyl- \mathcal{N} -(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191939-92-1 CA

CN 4-Quinolinecarboxamide, 3-[(dimethylamino)methyl]-2-phenyl- \mathcal{N} -(1-phenylpropyl)-, monohydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE

63

191939-92-1 CA

• HCI

Copyright © 1997 American Chemical Society (ACS)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

64

L6 ANSWER 4 OF 17 CA COPYRIGHT 1997 ACS

DUPLICATE 4

AN 127:95204 CA

TI Preparation of quinoline-4-carboxamides and their use as neurokinin-3 and neurokinin-2 receptor antagonists

IN Giardina, Giuseppe Arnaldo Maria; Grugni, Mario; Raveglia, Luca Francesco; Farina, Carlo

PA Smithkline Beecham S.P.A., Italy; Giardina, Giuseppe Arnaldo Maria; Grugni, Mario; Raveglia, Luca Francesco; Farina, Carlo

SO PCT Int. Appl., 79 pp. CODEN: PIXXD2

PI WO 9719926 A1 970605

DS TT, W UA, W UG, W US, W UZ, W VN, W AM, W AZ, W BY, W KG, W KZ, W MD, W RU, W TJ, W TM, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG

AI WO 96-EP5207 961122 PRAI IT 95-MI2462 951124

IT 96-MI1688 960802

DT Patent

LA English

OS MARPAT 127:95204

GI

$$\begin{array}{c|c}
R^4 & A \\
\hline
0 & NH & R^2 \\
R^1 & & & \\
R^3 & & & \\
\end{array}$$

The title compds. [I; A = (un)substituted aryl, C_{5-7} cycloalkdienyl, (un)substituted single or fused ring arom. heterocyclyl; R = (un)substituted C_{1-6} alkyl, C_{3-7} cycloalkylalkyl, (un)substituted Ph, an optionally substituted five-membered heteroarom. ring, etc.; R^1 = hydrogen or up to four substituents selected from C_{1-6} alkyl, C_{1-6} alkenyl, aryl, C_{1-6} alkoxy, hydroxy, halogen, nitro, cyano, carboxy, carboxamido, sulfonamido, C_{1-6} alkoxycarbonyl, trifluoromethyl, alkoxy, phthalimido, (un)substituted amino, etc.; R^2 = hydrogen, C_{1-6} alkyl, hydroxy, halogen, cyano, (un)substituted amino, etc.; R^3 = C_{1-6} alkyl, C_{3-7} cycloalkyl, C_{4-7} cycloalkylalkyl, (un)substituted aryl, (un)substituted single or fused ring arom. heterocyclyl; R^4 = hydrogen, C_{1-6} alkyl, useful as neurokinin 3 and neurokinin 2 receptor antagonists, are prepd.

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

65

L6 ANSWER 4 OF 17 CA COPYRIGHT 1997 ACS.

DUPLICATE 4

Thus, $(S)-N-(\alpha-\text{ethylbenzyl})-3-(2-\text{aminoethoxy})-2-\text{phenylquinoline}-4-\text{carboxamide}$ was reacted with α,α' -dibromo-o-xylene and salified with HCl, producing $(S)-N-(\alpha-\text{ethylbenzyl})-3-[2-(2-\text{isoindolinyl})\text{ethoxy}]-2-\text{phenylquinoline}-4-\text{carboxamide}$ dihydrochloride

(S)-N-(α -ethylbenzyl)-3-[2-(2-isoindolinyl)ethoxy]-2-phenylquinoline-4-carboxamide dihydrochloride (m.p. 95°; decompn.) which demonstrated a binding affinity in human neurokinin-3 receptors (expressed in CHO cell lines) against [^{125}I]-[Me-Phe 7]-neurokinin B of 1.2 nM.

P*** ***191796-43-7P*** ***191796-44-8P*** ***191796-45-9P***

191796-46-0P ***191796-47-1P*** ***191796-48-2P*** ***191796-49-3

P*** ***191796-50-6P*** ***191796-51-7P*** ***191796-52-8P***

P*** ***191796-57-3P*** ***191796-58-4P*** ***191796-59-5P***

P*** ***191796-64-2P*** ***191796-65-3P*** ***191796-66-4P***

191796-67-5P** ***191796-68-6P ***191796-69-7P** ***191796-70-0

P***

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of quinoline-4-carboxamides and their use as neurokinin-3 and neurokinin-2 receptor antagonists)

RN 191796-25-5 CA

CN 4-Quinolinecarboxamide, 3-(4-morpholinylmethyl)-2-phenyl-N-(1-phenylpropyl)-, monohydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

• HCI

RN 191796-26-6 CA

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

66

RN 191796-26-6 CA

NAME)

CN 4-Quinolinecarboxamide, $3-(2-hydroxyethoxy)-2-phenyl-\mathcal{N}-(1-phenylpropyl)-$, (S)- (9CI)

(CA INDEX

Absolute stereochemistry. Rotation (-).

RN 191796-27-7 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-7-methyl-2-phenyl-/V-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 191796-28-8 CA

CN 4-Quinolinecarboxamide, 3-fluoro-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

RN 191796-29-9 CA

CN 4-Quinolinecarboxamide, 3-[2-(1,3-dihydro-2*H*-isoindol-2-yl)ethoxy]-2-phenyl-*N*-(1-phenylpropyl)-, dihydrochloride, (*S*)- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

67

RN 191796-29-9 CA Absolute stereochemistry.

• 2 HCI

RN 191796-30-2 CA

CN 4-Quinolinecarboxamide,

3-[2-(3,4-dihydro-1,3-dioxo-2(1H)-isoquinolinyl)ethoxy]-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-31-3 CA

CN 4-Quinolinecarboxamide, 3-[2-(3,4-dihydro-2(1//)-isoquinolinyl)ethoxy]-2-phenyl-/V-(1-phenylpropyl)-, monohydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

68

RN 191796-31-3 CA

• HCI

RN 191796-32-4 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-/V-(2-oxo-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 191796-33-5 CA

CN 4-Quinolinecarboxamide,

3-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)propoxy]-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-34-6 CA

CN 4-Quinolinecarboxamide,

 $3-[2-(3,4-dihydro-3-hydroxy-1-oxo-2(1/H)-isoquinolinyl)ethoxy]-2-phenyl-<math>\mathcal{N}-(1-phenylpropyl)-$, [2(S)]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE

69

RN 191796-34-6 CA

191796-35-7 RN CA

4-Quinolinecarboxamide, 3-(3-aminopropoxy)-2-phenyl-N-(1-phenylpropyl)-, monohydrochloride, (S)-CN (CA INDEX NAME) (9CI)

Absolute stereochemistry. Rotation (-).

HCI

191796-36-8 CA RN

 $4- Quinoline carboxamide, \quad 3- [2-(1-oxo-2(1H)-isoquinolinyl)ethoxy] - 2-phenyl-\mathcal{N}-(1-phenylpropyl)-, \quad (S)-(1-oxo-2(1H)-isoquinolinyl)ethoxy] - 2-phenyl-\mathcal{N}-(1-oxo-2(1H)-isoquinolinyl)ethoxy] - 2-phenyl-\mathcal{N}-(1-oxo-2(1H)-isoquinolinyl)eth$ CN (CA INDEX NAME) (9CI)

Absolute stereochemistry. Rotation (+).

191796-37-9 CA RN

 $4- Quino line carboxamide, 2- phenyl- \mathcal{N}-(1- phenyl propyl)-3-[[(1- phenyl propyl) amino] methyl]-, \\$ CN monohydrochloride, [S-(R*,R*)]-(9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

70

RN - 191796-37-9 CA

Absolute stereochemistry. Rotation (-).

• HCI

RN 191796-38-0 CA

CN 4-Quinolinecarboxamide,

3-[2-(3,4-dihydro-3-oxo-2(1H)-isoquinolinyl)ethoxy]-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-39-1 CA

CN 4-Quinolinecarboxamide, $3-[2-(2,5-\text{diox}o-1-\text{pyrrolidinyl})\text{ethoxy}]-2-\text{phenyl-}\mathcal{N}-(1-\text{phenylpropyl})-$, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-40-4 CA

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

71

RN 191796-40-4 CA

CN 4-Quinolinecarboxamide,

3-[2-(2,5-dihydro-2,5-dioxo-1H-pyrrol-1-yl)ethoxy]-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-41-5 CA

CN 4-Quinolinecarboxamide,

3-[2-(2,2-dimethyl-5-oxo-1-imidazolidinyl)ethoxy]-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-42-6 CA

CN 4-Quinolinecarboxamide,

3-[3-[4-(2-methoxyphenyl)-1-piperazinyl]propoxy]-2-phenyl-\$N-(1-phenylpropyl)-, dihydrochloride, (S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

72

RN 191796-42-6 CA

• 2 HCI

RN 191796-43-7 CA

CN 4-Quinolinecarboxamide, 3-[2-(5-oxo-2-phenyl-1-imidazolidinyl)ethoxy]-2-phenyl-<math>N-(1-phenylpropyl)-, [1(S)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 191796-44-8 CA

CN 4-Quinolinecarboxamide,

3-[2-(2,2-dimethyl-5-oxo-4-phenyl-1-imidazolidinyl)ethoxy]-2-phenyl-\$N-(1-phenylpropyl)-, [\$S-(\$R*,\$R*)]-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-45-9 CA

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

73

RN 191796-45-9 CA

CN 4-Quinolinecarboxamide,

 $3-[2-(2,2-dimethyl-5-oxo-4-phenyl-1-imidazolidinyl)ethoxy]-2-phenyl-$\mathcal{N}-(1-phenylpropyl)-, [$S-($R*,$S*)]-(9CI) (CA INDEX NAME)$

Absolute stereochemistry. Rotation (-).

RN 191796-46-0 CA

CN 4-Quinolinecarboxamide,

3-[2-(3,4-dihydro-1-oxo-2(1H)-isoquinolinyl)ethoxy]-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-47-1 CA

CN 4-Quinolinecarboxamide, 3-[[methyl(phenylmethyl)amino]methyl]-2-phenyl-N-(1-phenylpropyl)-, (S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-48-2 CA

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

74

RN 191796-48-2 CA

CN 4-Quinolinecarboxamide, 3-methyl- \mathcal{N} -(2-oxo-1-phenylpropyl)-2-phenyl-, (-)- (9CI) (CA INDEX NAME)

Rotation (-).

RN 191796-49-3 CA

CN 4-Quinolinecarboxamide, 3-methyl-N-(2-oxo-1-phenylpropyl)-2-phenyl-, (+)- (9CI) (CA INDEX NAME)

Rotation (+).

RN 191796-50-6 CA

CN Benzeneacetic acid, α -methyl- α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 191796-51-7 CA

CN Benzeneacetic acid, α -methyl- α -[[(3-methyl-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57 PAGE RN 191796-51-7 CA

75

RN 191796-52-8 CA

CN 4-Quinolinecarboxamide, 3-methyl-N-(1-methyl-2-oxo-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 191796-53-9 CA

CN 4-Quinolinecarboxamide, 3-[(methyl-2-propenylamino)methyl]-2-phenyl- \mathcal{N} -(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-54-0 CA

CN 4-Quinolinecarboxamide, 2-phenyl-3-[(4-phenyl-1-piperazinyl)methyl]- \mathcal{N} -(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

76

RN 191796-54-0 CA

RN 191796-55-1 CA

CN 4-Quinolinecarboxamide, $3-[3-(4-methyl-1-piperazinyl)propoxy]-2-phenyl-<math>\mathcal{N}-(1-phenylpropyl)-$, trihydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

• 3 HCI

RN 191796-56-2 CA

CN 4-Quinolinecarboxamide, 3-[3-[4-(2-chlorophenyl)-1-piperazinyl]propoxy]-2-phenyl-<math>N-(1-phenylpropyl)-, dihydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

• 2 HCI

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

77

RN 191796-57-3 CA

RN 191796-57-3 CA

CN 4-Quinolinecarboxamide, 2-phenyl-3-[3-(4-phenyl-1-piperazinyl)propoxy]-N-(1-phenylpropyl)-, hydrochloride (2:5), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

• 5/2 HCI

RN 191796-58-4 CA

CN 4-Quinolinecarboxamide, 3-[3-[4-(3-chlorophenyl)-1-piperazinyl]propoxy]-2-phenyl-N-(1-phenylpropyl)-, dihydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

2 HCI

RN 191796-59-5 CA

CN 4-Quinolinecarboxamide, 3-[3-[4-(4-chlorophenyl)-1-piperazinyl]propoxy]-2-phenyl-/V-(1-phenylpropyl)-, dihydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE

78

RN 191796-59-5 CA

• 2 HCI

RN 191796-60-8 CA

CN 4-Quinolinecarboxamide,

> 3-[3-[4-(4-methoxyphenyl)-1-piperazinyl]propoxy]-2-phenyl-N-(1-phenylpropyl)-, dihydrochloride, (S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

• 2 HCI

RN 191796-61-9 CA

CN $4- Quino line carboxamide, \quad 3-[3-[4-(4-methylphenyl)-1-piperazinyl] propoxy] -2-phenyl- \mathcal{N}-(1-phenylpropyl)-,$ hydrochloride (2:5), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C RN 191796-61-9 CA

08 OCT 1997 20:02:57

PAGE

79

• 5/2 HCI

RN 191796-62-0 CA

CN 1-Piperazinecarboxylic acid,

4-[3-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]propyl]-, 1,1-dimethylethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-63-1 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-(1-phenylpropyl)-3-[3-(1-piperazinyl)propoxy]-, trihydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

• 3 HCI

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

80

RN 191796-63-1 CA

RN 191796-64-2 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-(1-phenylpropyl)-3-[3-[4-(2-pyrimidinyl)-1-piperazinyl]propoxy]-, hydrochloride (2:5), (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

• 5/2 HCI

RN 191796-65-3 CA

CN 4-Quinolinecarboxamide, 3-[3-(3-azaspiro[5.5]undec-3-yl)propoxy]-2-phenyl-<math>N-(1-phenylpropyl)-, monohydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

• HCI

RN 191796-66-4 CA

CN 4-Quinolinecarboxamide,

3-[3-(5,7-dihydro-5,7-dioxo-6H-pyrrolo[3,4-b]pyrazin-6-yl)propoxy]-2-phenyl-N-(1-phenylpropyl)-, (S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-67-5 CA

CN 4-Quinolinecarboxamide, 3-(1H-imidazol-1-ylmethyl)-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-68-6 CA

CN 4-Quinolinecarboxamide, 2-phenyl-3-[2-[(phenylmethyl)amino]ethoxy]-N-(1-phenylpropyl)-, monohydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

HCI

RN 191796-69-7 CA

CN 4-Quinolinecarboxamide, 3-[2-[bis(phenylmethyl)amino]ethoxy]-2-phenyl-N-(1-phenylpropyl)-, monohydrochloride, (S)- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

82

RN 191796-69-7 CA

Absolute stereochemistry. Rotation (-).

HCI

RN 191796-70-0 CA

CN 4-Quinolinecarboxamide, 2-phenyl-3-[2-[(2-phenylethyl)amino]ethoxy]- \mathcal{N} -(1-phenylpropyl)-, monohydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

• HCI

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

(prepn. of quinoline-4-carboxamides and their use as neurokinin-3 and neurokinin-2 receptor antagonists)

RN 174636-32-9 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl- \mathcal{N} -(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

Copyright © 1997 American Chemical Society (ACS)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

83

RN 174636-32-9 CA

RN 191796-72-2 CA

Acetic acid, [[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]-, ethyl ester, (S)-CN (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-73-3 CA

CN 4-Quinolinecarboxamide,

> 3-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethoxy]-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI)INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-74-4 CA

CN 4-Quinoline carboxamide, 3-(2-aminoethoxy)-2-phenyl-<math>N-(1-phenylpropyl)-, (S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

84

RN 191796-74-4 CA

RN 191796-75-5 CA

CN 4-Quinolinecarboxamide, 3-(2-oxoethoxy)-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 191796-76-6 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-N-(2-hydroxy-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 191796-77-7 CA

CN 4-Quinolinecarboxamide,

3-[2-[[[2-(hydroxymethyl)phenyl]acetyl]amino]ethoxy]-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-78-8 CA

CN Butanoic acid,

4-oxo-4-[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-79-9 CA

CN 2-Butenoic acid,

4-oxo-4-[[2-[[2-phenyl-4-[[(1-phenylpropyl)amino]carbonyl]-3-quinolinyl]oxy]ethyl]amino]-, [S-(Z)]-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

RN 191796-80-2 CA

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

86

RN 191796-80-2 CA

CN 4-Quinolinecarboxamide, 3-[2-[(aminoacetyl)amino]ethoxy]-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-81-3 CA

CN 4-Quinolinecarboxamide, $3-[2-[(aminophenylacetyl)amino]ethoxy]-2-phenyl-$\mathcal{N}-(1-phenylpropyl)-, [$S-($R*,$R*)]- (9CI) (CA INDEX NAME)$

Absolute stereochemistry. Rotation (-).

RN 191796-82-4 CA

CN 4-Quinolinecarboxamide, 3-[2-[(aminophenylacetyl)amino]ethoxy]-2-phenyl-N-(1-phenylpropyl)-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 191796-88-0 CA

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE

87

RN 191796-88-0 CA

CN NAME)

Copyright © 1997 American Chemical Society (ACS)

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE

88

L6 ANSWER 5 OF 17 CA COPYRIGHT 1997 ACS

DUPLICATE 5

AN 126:338400

TI Discovery of a Novel Class of Selective Non-Peptide Antagonists for the Human Neurokinin-3 Receptor. 1. Identification of the 4-Quinolinecarboxamide Framework

ΑU Giardina, Giuseppe A. M.; Sarau, Henry M.; Farina, Carlo; Medhurst, Andrew D.; Grugni, Mario; Raveglia, Luca F.; Schmidt, Dulcie B.; Rigolio, Roberto; Luttmann, Mark; et al.

CS Department of Chemistry, SmithKline Beecham S.p.A., Baranzate, 20021, Italy

SO J. Med. Chem. (1997), 40(12), 1794-1807 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

OS CJACS-IMAGE: CJACS

AB A novel class of potent and selective non-peptide neurokinin-3 (NK-3) receptor antagonists, featuring the 4-quinolinecarboxamide framework, was designed based upon chem. diverse NK-1 The novel compds., prompted by chem. modifications of the prototype, receptor antagonists. were characterized by binding anal, using a membrane prepn. of chinese hamster ovary (CHO) cells expressing the human neurokinin-3 receptors (hNK-3-CHO), and clear structure-activity relationships (SARs) were established. From SARs,

(R)-N-[α -(methoxycarbonyl)benzyl]-2-phenylquinoline-4-carboxamide (I, SB 218795, hNK-3-CHO binding $K_i = 13$ nM) emerged as one of the most potent compds. of this novel class. Selectivity studies vs. the other neurokinin receptors (hNK-2-CHO and hNK-1-CHO) revealed that 65 is about 90-fold selective for hNK-3 vs. hNK-2 receptors (hNK-2-CHO binding K_i = 1221 nM) and over 7000-fold selective vs. hNK-1 receptors (hNK-1-CHO binding $K_i = >100$ μ M). In vitro functional studies in rabbit isolated iris sphincter muscle prepn. demonstrated that I a competitive antagonist of the contractile response induced by the potent and selective NK-3 receptor agonist senktide with a $K_b = 43$ nM. Overall, the data indicate that I is a potent and selective hNK-3 receptor antagonist and a useful lead for further chem. optimization.

```
IT
      ***174635-51-9P***
                                ***174635-52-0P***
                                                         ***174635-53-1P*** , SB 218795
      ***174635-54-2P***
                                ***174635-56-4P***
                                                         ***174635-58-6P***
                                                                                   ***174635-59-7
                  ***174635-60-0P***
                                           ***174635-61-1P***
                                                                    ***174635-71-3P***
                                ***174635-91-7P***
      ***174635-73-5P***
                                                         ***174635-97-3P***
                                                                                  ***174635-98-4
```

174636-00-1P ***174636-01-2P*** ***174636-04-5P***

174636-06-7P ***174636-07-8P*** ***174636-09-0P*** ***174636-13-6

174636-23-8P ***174636-24-9P*** . ***174636-25-0P***

174636-40-9P ***189815-88-1P*** ***189815-93-8P*** ***189815-94-9 P***

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. of quinolinecarboxamide-contg. nonpeptide neurokinin-3 receptor antagonists)

RN 174635-51-9 CA

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

89

RN 174635-51-9 CA

CN Benzeneacetic acid, α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-52-0 CA

CN Benzeneacetic acid, α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 174635-53-1 CA

CN Benzeneacetic acid, α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 174635-54-2 CA

CN Benzeneacetic acid, α -[[(7-methoxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

INTERNATIONAL®

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE

90

RN 174635-54-2 CA

RN 174635-56-4

CN Benzeneacetic acid, α -[[(7-methoxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)

• HCI

RN 174635-58-6

CN Benzeneacetic acid, α -[[[2-(2-thienyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) INDEX NAME)

RN 174635-59-7

CN Benzeneacetic acid, α -[[[2-(2-furanyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) INDEX NAME) -

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

91

RN 174635-59-7 CA

RN 174635-60-0

Benzeneacetic acid, α -[[[2-(4-pyridinyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) CN INDEX NAME)

RN 174635-61-1 CA

2-Thiopheneacetic acid, α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) CN (CA INDEX NAME)

RN 174635-71-3 CA

Benzeneacetic acid, α -[[[2-(2-methoxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) CN (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE

92

RN 174635-71-3 CA

RN 174635-73-5 CA

Benzeneacetic acid, α -[[[2-(2-fluorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) CN (CA INDEX NAME)

RN 174635-91-7 CA

Benzeneacetic acid, α -[[[2-(2-benzofuranyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) CN (CA INDEX NAME)

RN 174635-97-3 CA

CN Benzeneacetic acid, α -[methyl[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

93

RN 174635-97-3 CA

RN 174635-98-4

Benzeneacetic acid, α -[[[2-(3-thienyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) CN INDEX NAME)

RN 174636-00-1 CA

Benzeneacetic acid, α -[[[2-(1H-pyrrol-2-yl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) CN (CA INDEX NAME)

RN 174636-01-2 CA

CN Benzeneacetic acid, α -[[[2-(2-thiazolyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

94

RN 174636-04-5 CA

RN 174636-04-5 CA

CN Benzeneacetic acid, α -[[[2-(4-methylphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-06-7 CA

CN Benzeneacetic acid, α -[[[2-(2-methylphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-07-8 CA

CN Benzeneacetic acid, α -[[[2-(4-methoxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-09-0 CA

CN Benzeneacetic acid, α -[[[2-(4-hydroxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

INTERNATIONAL®

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 95

RN 174636-09-0 CA

RN 174636-13-6 CA

Benzeneacetic acid, α -[[[2-(1H-pyrrol-3-yl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) CN (CA INDEX NAME)

RN 174636-23-8 CA

Benzeneacetic acid, α -[[(2-cyclohexyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) CN INDEX NAME)

RN 174636-24-9 CA

Benzeneacetic acid, α -[[[2-(3-chlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) CN (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

96

RN 174636-24-9 CA

RN 174636-25-0 CA

CN Benzeneacetic acid, α -[[[2-(2-chlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-40-9 CA

CN Benzeneacetic acid, α -[[[2-(4-chlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 189815-88-1 CA

CN Benzeneacetic acid, α -[[[2-(2-hydroxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 189815-93-8 CA

CN Benzeneacetic acid, 4-hydroxy- α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE

97

RN 189815-93-8 CA

RN 189815-94-9 CA

Benzeneacetic acid, 4-methoxy- α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (R)-CN (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Copyright © 1997 American Chemical Society (ACS)

COPYRIGHT 1997 ACS CA

DUPLICATE 6

ANSWER 6 OF 17 L6

Nonpeptide tachykinin receptor antagonists: I. Pharmacological and pharmacokinetic ΑN

characterization of SB 223412, a novel, potent and selective neurokinin-3 receptor antagonist

Sarau, Henry M.; Griswold, Don E.; Potts, William; Foley, James J.; Schmidt, Dulcie B.; TI ΑU

Webb, Edward F.; Martin, Lenox D.; Brawner, Mary E.; Elshourbagy, Nabil A.; Medhurst,

Andrew D.; Giardina, Giuseppe A. M.; Hay, Douglas W. P.

Departments of Pulmonary Pharmacology, Immunopharmacology, Drug Metabolism and Pharmacokinetics, Gene Expression Sciences and Molecular Genetics, SmithKline Beecham CS Pharmaceuticals, King of Prussia, PA, 19406, USA

J. Pharmacol. Exp. Ther. (1997), 281(3), 1303-1311 **SO**

CODEN: JPETAB; ISSN: 0022-3565

Williams & Wilkins PB

Journal Ta

LA

AB

The in vitro and in vivo pharmacol. profile of SB 223412 [(S)-(-)-N-(α -ethylbenzyl)-3-hydroxy-2-phenylquinoline-4-carboxamide], a novel human NK-3 English (hNK-3) receptor antagonist, is described. SB 223412 demonstrated enantioselective affinity for inhibition of [125] [MePhe7] neurokinin B (NKB) binding to membranes of CHO cells expressing the hNK-3 receptor (CHO hNK-3). SB 223412, the (S)-isomer, ($K_i = 1.0$ nM), has similar affinity as the natural ligand, NKB (K_i = 0.8 nM) and another nonpeptide NK-3 receptor antagonist, SR 142801 ($K_i = 1.2$ nM). receptors compared with hNK-1 (>10,000-fold selective) and hNK-2 receptors (>140-fold selective), and selectivity was further demonstrated by its lack of effect, in concns. up to SB 223412 enantioselectively 1 or 10 μ M, in >60 receptor, enzyme and ion channel assays. inhibited the NKB-induced Ca++ mobilization in HEK 293 cells stably expressing the hNK-3 SB 223412 (10-1,000 nM) produced concn.-dependent rightward shifts in NKB-induced CA^{++} mobilization concn.-response curves with a K_b value of 3 nM. antagonized senktide-induced contraction in the isolated rabbit iris sphincter muscle (K_b = 1.6 In mice, oral administration of SB 223412 produced dose-dependent inhibition of behavioral responses induced by the NK-3 receptor-selective agonist, senktide (ED $_{50}$ = 12.2 Pharmacokinetic evaluation of SB 223412 in rat and dog indicted low plasma clearance, oral bioavailability and high and sustained plasma concns. after 4 to 8 mg/kg oral The preclin. profile of SB 223412 (high affinity, selectivity, reversibility and oral activity) suggests that it will be a useful tool compd. to define the physiol. and pathophysiol. roles of NK-3 receptors.

IT

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BIOL ***174636-32-9*** (Biological study); PROC (Process)

(pharmacol. and pharmacokinetic characterization of NK-3 antagonist SB 223412)

RN

4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX CN

American Chemical Society (ACS) Copyright © 1997

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE

99

RN 174636-32-9 CA

Absolute stereochemistry. Rotation (-).

Copyright © 1997 American Chemical Society (ACS)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 100

L6 ANSWER 7 OF 17 CA COPYRIGHT 1997 ACS

DUPLICATE 7

AN 127:4735 CA

Direct tritium labeling of multifunctional compounds using organoiridium catalysis TI

Chen, W.; Garnes, K.T.; Levinson, S.H.; Saunders, D.; Senderoff, S.G.; Shu, A.Y.L.; Villani, A.J.; ΑU CS

Radiochemistry, SmithKline Beecham Pharmaceuticals, King of Prussia, PA, 19406, USA

SO J. Labelled Compd. Radiopharm. (1997), 39(4), 291-298 CODEN: JLCRD4; ISSN: 0362-4803 PB

Wiley

DT Journal

LA English

AB The tritium exchange labeling of a variety of complex compds. is achieved in the presence of catalyst precursor $[(cod)Ir(PPh_3)_2]BF_4$ and limited amts. of tritium gas. of exchange is high and consistent with empirical rules previously obsd. The regioselectivity activity levels are often achieved, usually with specific aryl C-H bonds. High specific remarkably efficient exchange occurs in certain N-alkyl groups. However, Studies of intermol. inhibition of catalytic exchange suggest reasons why larger amts. of complex are sometimes required to label complex mols.; nevertheless, significant amts. of label incorporation into substrates can be achieved even starting with small amts. of labeling gas. IT ***174636-26-1DP***

, deuterated

RL: SPN (Synthetic preparation); PREP (Preparation)

(direct deuterium labeling of multifunctional compds. using organoiridium catalysts)

RN 174636-26-1

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

IT ***174636-26-1***

RL: RCT (Reactant)

(direct tritium labeling of multifunctional compds. using organoiridium catalysts)

RN 174636-26-1

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 101

RN 174636-26-1 CA

IT ***190187-74-7P***

RL: SPN (Synthetic preparation); PREP (Preparation)

(direct tritium labeling of multifunctional compds. using organoiridium catalysts)

RN 190187-74-7 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-(phenyl- $2,6-t_2$)- \mathcal{N} -(1-phenylpropyl)- (9CI) (CA INDEX NAME)

IT ***174635-78-0***

RL: RCT (Reactant)

(inhibition of Et benzoate deuteration by dioxa compds.)

RN 174635-78-0 CA

CN 4-Quinolinecarboxamide, 3-methyl-2-phenyl-/V-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

IT ***174635-78-0DP*** , deuterated

RL: SPN (Synthetic preparation); PREP (Preparation)

(inhibition of Et benzoate deuteration by dioxa compds.)

RN 174635-78-0 CA

CN 4-Quinolinecarboxamide, 3-methyl-2-phenyl-/V-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

Copyright © 1997 American Chemical Society (ACS)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

104

RN 185508-92-3 CA

RN 185508-92-3 CA

CN (CA INDEX NAME)

Absolute stereochemistry.

Copyright © 1997 American Chemical Society

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE 105

L6 ANSWER 9 OF 17 CA COPYRIGHT 1997 ACS **DUPLICATE 9**

AN 125:25636 CA

TI 2-Phenyl-4-quinolinecarboxamides: A Novel Class of Potent and Selective Non-Peptide Competitive Antagonists for the Human Neurokinin-3 Receptor

AU Giardina, Giuseppe A. M.; Sarau, Henry M.; Farina, Carlo; Medhurst, Andrew D.; Grugni, Mario; Foley, James J.; Raveglia, Luca F.; Schmidt, Dulcie B.; Rigolio, Roberto; et al.

CS Department of Chemistry, SmithKline Beecham S.p.A., Baranzate, 20021, Italy

S0 J. Med. Chem. (1996), 39(12), 2281-2284 CODEN: JMCMAR; ISSN: 0022-2623

DT **Journal**

LA English

OS CJACS-IMAGE: CJACS

AB A novel class of potent and selective, non-peptide NK-3 receptor antagonists, based on the 2-phenylquinoline framework, has been identified and characterized by binding anal. using membrane prepn. of CHO cells expressing the human neurokinin receptors (hNKs-CHO). Functional activity was detd. by inhibition of senktide-induced contraction of the rabbit isolated iris sphincter muscle prepn. An extensive structure-activity study led to the identification of $(S)-(-)-N-(\alpha-\text{ethylbenzyl})-3-\text{hydroxy}-2-\text{phenylquinoline}-4-\text{carboxamide}$ (SB 223412) as the most potent ($K_i = 1.0$ nm in hNK-3-CHO binding; $K_b = 5.4$ nM for antagonism of senktide-induced contraction in rabbit iris sphincter muscle) and selective (hNK-2/hNK-3 Ki ratio of 144 and hNK-1/hNK-3 K_i ratio > 100,000) hNK-3 receptor antagonist of this class. In addn., NKB-induced Ca²⁺ mobilization studies in hNK-3-HEK 293 cells indicated that SB Compds. from this novel class will be 223412 is a reversible, competitive antagonist. extremely useful in the functional characterization of hNK-3 receptors and elucidation of potential therapeutic indications for selective hNK-3 receptor antagonists.

174635-51-9P IT

174635-52-0P

174635~53~1P

***174635-69-9

174636-20-5P

174636-32-9P , SB 223412

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and structure-activity of human neurokinin 3 receptor antagonists phenylquinolinecarboxamides)

RN 174635-51-9

Benzeneacetic acid, α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX CN NAME)

Copyright @ 1997 American Chemical Society (ACS)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 106

RN 174635-52-0 CA

RN 174635-52-0 CA

CN Benzeneacetic acid, α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 174635-53-1 CA

CN Benzeneacetic acid, α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 174635-69-9 CA

CN 4-Quinolinecarboxamide, 3-methyl-2-phenyl- \mathcal{N} -(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

RN 174636-20-5 CA

CN 4-Quinolinecarboxamide, 2-phenyl- \mathcal{N} -(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE 107

RN 174636-20-5 CA

174636-32-9 CA RN

CN Absolute stereochemistry. Rotation (-).

Copyright © 1997 American Chemical Society (ACS)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 108

L6 ANSWER 10 OF 17 CA COPYRIGHT 1997 ACS

DUPLICATE 10

AN 124:232269 CA

TI Quinoline derivatives as tachykinin NK₃ receptor antagonists

IN Farina, Carlo; Giardina, Giuseppe Arnaldo Mari; Grugni, Mario; Raveglia, Luca Francesco

PA Smithkline Beecham Farmaceutici S.P.A., Italy

SO PCT Int. Appl., 95 pp.

CODEN: PIXXD2

PI WO 9532948 A1 951207

DS W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT

RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG

AI WO 95-EP2000 950523

PRAI IT 94-MI1099 940527

IT 95-MI494 950314

DT Patent

LA English

OS MARPAT 124:232269

GI

NK₃ receptor antagonists I [Ar = (un)substituted Ph, naphthyl, cycloalkadienyl, heteroaryl; R = (un)substituted alkyl, cycloalkyl, (un)substituted Ph, phenylalkyl, or heteroaryl, CO_2H and derivs., etc.; R¹, R² = H, alkyl; or R¹R² = (CH_2)₃₋₅; or RR¹ = (CH_2)₂₋₅; R³, R⁴ = H, alkyl, alkenyl, aryl, alkoxy, OH, halo, NO₂, amino, etc.; R⁵ = alkyl, cycloalkyl, (un)substituted (hetero)aryl; X = O, S, N(CN)] are useful in treating pulmonary, CNS, and neurodegenerative disorders, etc. Approx. 115 compds. were prepd. For example, amidation of 3-methyl-2-phenylquinoline-4-carbonyl chloride with (R)- α -ethylbenzylamine gave title compd. II in 58% yield. II had IC50 of 5.6 nM for displacement of [³H]-senktide from guinea-pig cortical NK₃ receptors. Antagonist activity of I was shown by inhibition of senktide-induced contraction of guinea-pig ileum.

IT ***174635-48-4P***

174635-49-5P

174635-50-8P

***174635-51-9

P***

174635-52-0P

174635-53-1P

174635-54-2P

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE 109

```
L6
       ANSWER 10 OF 17 CA COPYRIGHT 1997 ACS
                                                                        DUPLICATE 10
       ***174635-55-3P***
                                 ***174635-56-4P***
                                                           ***174635-57-5P***
                                                                                      ***174635-58-6
                   ***174635-59-7P***
                                             ***174635-60-0P***
                                                                       ***174635-61-1P***
       ***174635-62-2P***
                                 ***174635-63-3P***
                                                           ***174635-64-4P***
                                                                                      ***174635-65-5
       P***
                   ***174635-66-6P***
                                             ***174635-68-8P***
                                                                       ***174635-69-9P***
       ***174635-70-2P***
                                 ***174635-71-3P***
                                                           ***174635-72-4P***
                                                                                     ***174635-73-5
                   ***174635-74-6P***
                                             ***174635-75-7P***
                                                                       ***174635-76-8P***
       ***174635-77-9P***
                                 ***174635-78-0P***
                                                           ***174635-79-1P***
                                                                                     ***174635-80-4
                   ***174635-81-5P***
                                             ***174635-82-6P***
                                                                       ***174635-83-7P***
       ***174635-84-8P***
                                 ***174635-85-9P***
                                                            ***174635-86-0P***
                                                                                      ***174635-87-1
       P***
                   ***174635-88-2P***
                                             ***174635-89-3P***
                                                                       ***174635-90-6P***
       ***174635-91-7P***
                                 ***174635-92-8P***
                                                           ***174635-93-9P***
                                                                                     ***174635-94-0
      P***
                   ***174635-95-1P***
                                            ***174635-96-2P***
                                                                       ***174635-97-3P***
       ***174635-98-4P***
                                 ***174636-00-1P***
                                                           ***174636-01-2P***
                                                                                     ***174636-03-4
                   ***174636-04-5P***
                                             ***174636-05-6P***
                                                                       ***174636-06-7P***
       ***174636-07-8P***
                                 ***174636-09-0P***
                                                           ***174636-10-3P***
                                                                                     ***174636-11-4
      P***
                   ***174636-12-5P***
                                            ***174636-13-6P***
                                                                      ***174636-14-7P***
       ***174636-15-8P***
                                ***174636-16-9P***
                                                          ***174636-17-0P***
                                                                                    ***174636-18-1
      P***
                   ***174636-19-2P***
                                            ***174636-20-5P***
                                                                       ***174636-21-6P***
       ***174636-22-7P***
                                 ***174636-23-8P***
                                                           ***174636-24-9P***
                                                                                      ***174636-25-0
      P***
                   ***174636-26-1P***
                                            ***174636-27-2P***
                                                                       ***174636-28-3P***
      ***174636-29-4P***
                                 ***174636-30-7P***
                                                           ***174636-31-8P***
                                                                                     ***174636-32-9
                   ***174636-33-0P***
                                             ***174636-34-1P***
                                                                       ***174636-35-2P***
      ***174636-36-3P***
                                 ***174636-37-4P***
                                                           ***174636-38-5P***
                                                                                      ***174636-39-6
      P***
                   ***174636-40-9P***
                                                                       ***174636-42-1P***
                                             ***174636-41-0P***
      ***174636-43-2P***
                                 ***174636-44-3P***
                                                            ***174636-45-4P***
                                                                                      ***174636-46-5
      P***
                  ***174636~47-6P***
                                             ***174636-48-7P***
                                                                       ***174636-49-8P***
      ***174636-50-1P***
                                ***174636-51-2P***
                                                          ***174636-52-3P***
                                                                                    ***174636-53-4
                  ***174636-54-5P***
                                             ***174636-55-6P***
                                                                       ***174636-56-7P***
      ***174636-57-8P***
                                 ***174636-58-9P***
                                                           ***174636-59-0P***
                                                                                     ***174636-60-3
                  ***174636-61-4P***
                                            ***174636-62-5P***
       RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU
      (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
            (prepn. of quinolinecarboxamide derivs. as tachykinin NK3 receptor antagonists)
RN
       174635-48-4
                     CA
CN
       4-Quinolinecarboxamide, 2-phenyl-N-(1-phenylethyl)- (9CI) (CA INDEX NAME)
```

CA FILE SEARCH RESULTS - P281364C RN 174635-48-4 CA

08 OCT 1997 20:02:57

PAGE 110

RN 174635-49-5 CA

CN 4-Quinolinecarboxamide, 2-phenyl- \mathcal{N} -(1-phenylethyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (+).

RN 174635-50-8 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-(1-phenylethyl)-, (R)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

RN 174635-51-9 CA

CN Benzeneacetic acid, α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 111

RN 174635-52-0 CA

RN 174635-52-0 CA

CN Benzeneacetic acid, α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 174635-53-1 CA

CN Benzeneacetic acid, α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 174635-54-2 CA

CN Benzeneacetic acid, α -[[(7-methoxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-55-3 CA

CN Benzeneacetic acid, α -[[(7-hydroxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57.

PAGE 112

RN 174635-55-3 CA

RN 174635-56-4 CA

CN Benzeneacetic acid, α -[[(7-methoxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)

• HCI

RN 174635-57-5 CA

CN 4-Quinolinecarboxamide, N-[2-(methylamino)-2-oxo-1-phenylethyl]-2-phenyl- (9CI) (CA INDEX NAME)

RN 174635-58-6 CA

CN Benzeneacetic acid, α -[[[2-(2-thienyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C RN 174635-58-6 CA

08 OCT 1997 20:02:57

PAGE 113

S C-NH-CH-C-OMe

RN 174635-59-7 CA

CN Benzeneacetic acid, α -[[[2-(2-furanyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-60-0 CA

CN Benzeneacetic acid, α -[[[2-(4-pyridinyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-61-1 CA

CN 2-Thiopheneacetic acid, α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 114

RN 174635-61-1 CA

RN 174635-62-2 CA

CN Benzenepropanoic acid, β -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-63-3 CA

CN 1,4-Cyclohexadiene-1-acetic acid, α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 174635-64-4 CA

CN 4-Quinolinecarboxamide, N-(2-hydroxy-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME).

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 115

RN 174635-64-4 CA

RN 174635-65-5 CA

CN 4-Quinolinecarboxamide, 3-methoxy-2-phenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 174635-66-6 CA

CN 4-Quinolinecarboxamide, 3-butyl-2-phenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 174635-68-8 CA

CN 4-Quinolinecarboxamide, 3-hexyl-2-phenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 174635-69-9 CA

CN 4-Quinolinecarboxamide, 3-methyl-2-phenyl- \mathcal{N} -(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

PAGE 116

RN 174635-69-9 CA

RN 174635-70-2 CA

CN 4-Quinolinecarboxamide, 3-methyl-2-phenyl-N-(1-phenylpropyl)-, (R)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (+).

RN 174635-71-3 CA

CN Benzeneacetic acid, α -[[[2-(2-methoxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-72-4 CA

CN 4-Quinolinecarboxamide, 2,3-diphenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 117

RN 174635-72-4 CA

RN 174635-73-5 CA

CN Benzeneacetic acid, α -[[[2-(2-fluorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-74-6 CA

CN 4-Quinolinecarboxamide, N-[1-(3,4-dichlorophenyl)propyl]-2-phenyl- (9CI) (CA INDEX NAME)

RN 174635-75-7 CA

CN 4-Quinolinecarboxamide, N-(2-hydroxy-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 118

RN 174635-75-7 CA

RN 174635-76-8 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 174635-77-9 CA

CN Benzeneacetic acid, α -[[(3-methyl-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-78-0 CA

CN 4-Quinolinecarboxamide, 3-methyl-2-phenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 174635-79-1 CA

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 119

RN 174635-79-1 CA

CN Benzeneacetic acid, α -[[(7-chloro-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-80-4 CA

CN Benzeneacetic acid, α -[[(6-methyl-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-81-5 CA

CN 4-Quinolinecarboxamide, N-(2-methoxy-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 174635-82-6 CA

CN Benzeneacetic acid, α -[[(6-chloro-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE

120

RN 174635-82-6 CA

RN 174635-83-7 CA

CN Benzeneacetic acid, α -[[(3-ethyl-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-84-8 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-(1-phenylbutyl)- (9CI) (CA INDEX NAME)

RN 174635-85-9 CA

CN 4-Quinolinecarboxamide, 3-ethyl-2-phenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 174635-86-0 CA

CN 4-Quinolinecarboxamide, 3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-2-phenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE 121

174635-86-0 RN CA

174635-87-1 CA RN

CN 4-Quinolinecarboxamide, 2-phenyl-N-(1-phenylpropyl)-3-propyl- (9CI) (CA INDEX NAME)

RN 174635-88-2 CA

CN 4-Quinoline carboxamide, $6-bromo-2-(4-bromophenyl)-3-methyl-<math>\mathcal{N}-(1-phenylpropyl)-$, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 174635-89-3

CN 4-Quinolinecarboxamide, 6-bromo-3-methyl-2-phenyl-/V-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE 122

RN 174635-89-3 CA

CA RN 174635-90-6

Benzeneacetic acid, α -[[(6-methoxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) CN (CA INDEX NAME)

174635-91-7 CA RN

Benzeneacetic acid, α -[[[2-(2-benzofuranyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA CN INDEX NAME)

RN 174635-92-8 CA

4-Quinolinecarboxamide, N-(1,2-diphenylethyl)-2-phenyl- (9CI) (CA INDEX NAME) CN

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57 PAGE 123

RN 174635-93-9 CA CA RN 174635-93-9

CN 4-Quinolinecarboxamide, 2-phenyl-N-(2,2,2-trifluoro-1-phenylethyl)- (9CI) (CA INDEX NAME)

RN 174635-94-0 CA

4-Quinolinecarboxamide, 3-methoxy-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) CN Absolute stereochemistry. Rotation (-).

RN 174635-95-1 CA

CN 4-Quinolinecarboxamide, 3-ethyl-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

RN 174635-96-2

4-Quinolinecarboxamide, N-[1-(4-chlorophenyl)propyl]-2-phenyl- (9CI) (CA INDEX NAME) CN

CA FILE SEARCH RESULTS - P281364C RN 174635-96-2 CA

08 OCT 1997 20:02:57

PAGE 124

RN 174635-97-3 CA

CN Benzeneacetic acid, α -[methyl[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174635-98-4 CA

CN Benzeneacetic acid, α -[[[2-(3-thienyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-00-1 CA

CN Benzeneacetic acid, α -[[[2-(1H-pyrrol-2-yl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 125

RN 174636-00-1 CA

RN 174636-01-2 CA

CN Benzeneacetic acid, α -[[[2-(2-thiazolyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-03-4 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-(1-phenylpentyl)- (9CI) (CA INDEX NAME)

RN 174636-04-5 CA

CN Benzeneacetic acid, α -[[[2-(4-methylphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 126

RN 174636-05-6 CA

RN 174636-05-6 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-(1-phenyloctyl)- (9CI) (CA INDEX NAME)

RN 174636-06-7 CA

CN Benzeneacetic acid, α -[[[2-(2-methylphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-07-8 CA

CN Benzeneacetic acid, α -[[[2-(4-methoxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-09-0 CA

CN Benzeneacetic acid, α -[[[2-(4-hydroxyphenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 127

RN 174636-09-0 CA

RN 174636-10-3 CA

CN Benzeneacetic acid, α -[[[2-(1,3-benzodioxol-5-yl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-11-4 CA

CN 4-Quinolinecarboxamide, N-(1-methyl-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 174636-12-5 CA

CN 4-Quinolinecarboxamide, N-[1-(4-methylphenyl)propyl]-2-phenyl- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 128

RN 174636-12-5 CA

RN 174636-13-6 CA

Benzeneacetic acid, α -[[[2-(1H-pyrrol-3-yl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) CN INDEX NAME)

RN 174636-14-7 CA

Benzeneacetic acid, α -[[[2-(3,4-dichlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) CN (CA INDEX NAME)

RN 174636-15-8 CA

4-Quinolinecarboxamide, N-(2-amino-1-phenylethyl)-2-phenyl-, (R)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

RN 174636-16-9 CA

CN 4-Quinolinecarboxamide, 3-amino-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

RN 174636-17-0 CA

CN 4-Quinolinecarboxamide, 3-chloro-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

RN 174636-18-1 CA

CN 4-Quinolinecarboxamide, 3-bromo-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE 130

174636-18-1 CA RN

RN 174636-19-2 CA

CN 4-Quinolinecarboxamide, N-(2-methyl-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 174636-20-5 CA

4-Quinolinecarboxamide, 2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) CN Absolute stereochemistry. Rotation (-).

RN 174636-21-6 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-(1-phenylpropyl)-, (R)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (+).

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 131

RN 174636-22-7 CA

RN 174636-22-7 CA

CN Benzeneacetic acid, α -[[(6-fluoro-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-23-8 CA

CN Benzeneacetic acid, α -[[(2-cyclohexyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-24-9 CA

CN Benzeneacetic acid, α -[[[2-(3-chlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-25-0 CA

CN Benzeneacetic acid, α -[[[2-(2-chlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE 132

RN 174636-25-0 CA

RN 174636-26-1 CA

CN

4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-N-(1-phenylpropyl)- (9CI) (CA INDEX NAME)

RN 174636-27-2 CA

Benzeneacetic acid, α -[[[8-(acetyloxy)-2-phenyl-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) CN (CA INDEX NAME)

RN 174636-28-3 CA

Benzeneacetic acid, α -[[(8-hydroxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) CN (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 133

RN 174636-28-3 CA

RN 174636-29-4 CA

CN Benzeneacetic acid, α -[[[2-(2,4-dichlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-30-7 CA

CN Benzeneacetic acid, 4-hydroxy- α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, monohydrochloride, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

HCI

RN 174636-31-8 CA

CN 4-Quinolinecarboxamide, N-(diphenylmethyl)-2-phenyl- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 134

RN 174636-32-9 CA

RN 174636-32-9 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

RN 174636-33-0 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-2-phenyl-N-(1-phenylpropyl)-, (R)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (+).

RN 174636-34-1 CA

CN Benzeneacetic acid, α -[[(3-hydroxy-2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, (R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 174636-35-2 CA

CN 4-Quinolinecarboxamide, N-[2-(dimethylamino)-1-phenylethyl]-2-phenyl-, (R)- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 135

RN 174636-35-2 CA

Absolute stereochemistry. Rotation (-).

RN 174636-36-3 CA

CN 4-Quinolinecarboxamide, N-[2-(dimethylamino)-2-oxo-1-phenylethyl]-2-phenyl- (9CI) (CA INDEX NAME)

RN 174636-37-4 CA

CN 4-Quinolinecarboxamide, N-(2-amino-2-oxo-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 174636-38-5 CA

CN 4-Quinolinecarboxamide, N-[2-oxo-1-phenyl-2-(1-pyrrolidinyl)ethyl]-2-phenyl- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C RN 174636-38-5 CA

08 OCT 1997 20:02:57

PAGE 136

RN 174636-39-6 CA

CN Benzeneacetic acid, α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, monohydrochloride, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

HCI

RN 174636-40-9 CA

CN Benzeneacetic acid, α -[[[2-(4-chlorophenyl)-4-quinolinyl]carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-41-0 CA

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 137

RN 174636-41-0 CA

CN Benzeneacetic acid, 4-methoxy- α -[[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

RN 174636-42-1 CA

CN Benzeneacetic acid, α -methyl- α -[methyl[(2-phenyl-4-quinolinyl)carbonyl]amino]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

• HCI

RN 174636-43-2 CA

CN 4-Quinolinecarboxamide, N-(2-oxo-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 174636-44-3 CA

CN 4-Quinolinecarboxamide, N-(3-hydroxy-1-phenylpropyl)-2-phenyl- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE 138

174636-44-3 CA

RN 174636-45-4 CA

CN 4-Quinolinecarboxamide, $3-[2-(dimethylamino)ethoxy]-2-phenyl-$\times (1-phenylpropyl)-$\times (1-phenylpropylpropyl)-$\times (1-phenylpropylpropylpropylpropylpropyl)-$\times (1-phenylpropylpr$ monohydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

• HCI

RN 174636-46-5 CA

CN 4-Quinoline carboxamide, 3-(acetylamino)-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 174636-47-6 CA

CN 4-Quinolinecarboxamide, 3-[3-(dimethylamino)propoxy]-2-phenyl-/V-(1-phenylpropyl)-, monohydrochloride, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 139

RN 174636-47-6 CA

• HCI

RN 174636-48-7 CA

CN 4-Quinolinecarboxamide,

 $3-[2-(1,3-dihydro-1,3-dioxo-2\mathcal{H}-isoindol-2-yl)ethoxy]-2-phenyl-\mathcal{N}-(1-phenylpropyl)-, monohydrochloride, \\ (S)- (9CI) (CA INDEX NAME)$

Absolute stereochemistry. Rotation (-).

• HCI

RN 174636-49-8 CA

CN 4-Quinolinecarboxamide, 3-(2-aminoethoxy)-2-phenyl-N-(1-phenylpropyl)-, monohydrochloride, (S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE 140

RN 174636-49-8 CA

• HCI

RN 174636-50-1 CA

 $4- Quinoline carboxamide, 2-phenyl- \mathcal{N}-(1-phenylpropyl)-3-[2-(1-pyrrolidinyl)ethoxy]-, monohydrochloride, \\$ CN (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

· HCI

RN 174636-51-2 CA

CN 4-Quinolinecarboxamide, 3-[[(dimethylamino)acetyl]amino]-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE 141

RN 174636-52-3 CA

RN 174636-52-3 CA

CN 4-Quinolinecarboxamide, 3-hydroxy-/V-(1-methyl-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 174636-53-4 CA

CN 4-Quinolinecarboxamide, 3-amino-N-(1-methyl-1-phenylethyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 174636-54-5 CA

CN 4-Quinolinecarboxamide, 5-methyl-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME) Absolute stereochemistry. Rotation (-).

RN'174636-55-6 CA

CN 4-Quinolinecarboxamide, N-(2-hydroxy-1-phenylpropyl)-3-methyl-2-phenyl- (9CI) (CA_INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 142

174636-55-6 CA RN

RN 174636-56-7 CA

CN

RN 174636-57-8 CA

4-Quinoline carboxamide, $2-phenyl-\mathcal{N}-[1-(4-pyridinyl)propyl]-$ (9CI) (CA INDEX NAME) CN

RN174636-58-9 CA

CN 4-Quinolinecarboxamide, 2-phenyl-N-[1-(2-thienyl)propyl]- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 143

RN 174636-58-9 CA

RN 174636-59-0 CA

CN 4-Quinolinecarboxamide, 3-[(dimethylamino)methyl]-2-phenyl- \mathcal{N} -(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174636-60-3 CA

CN 4-Quinolinecarboxamide, 7-methoxy-3-methyl-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 174636-61-4 CA

CN 4-Quinolinecarboxamide, 3-amino-5-methyl-2-phenyl-/V-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE 144

RN 174636-61-4 CA

RN 174636-62-5 CA

CN 4-Quinolinecarboxamide, 3-methoxy-5-methyl-2-phenyl-N-(1-phenylpropyl)-, (S)- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 145

ANSWER 11 OF 17 CA COPYRIGHT 1997 ACS L6

DUPLICATE 11

AN 93:186338 CA

TI Ampicillin derivatives

PA Mitsubishi Yuka Yakuhin Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 10 pp.

CODEN: JKXXAF

PI JP 55055194 800422 Showa

ΑI JP 78-127324 781018

DT **Patent**

LA Japanese

GI

Fifteen title derivs. I (R = heterocyclic, heterocyclic-substituted methyl) were prepd. and the AB min. inhibition concns. treated against Ps. aeruginosa, St. aureus, B. substilis, E. coli, K1. pneumoniae, and Pr. vulgaris. Thus, 618 mg DCC was added to a mixt. of 648 4-carbamoyl-2-quinolinecarboxylic acid and 345 mg N-hydroxysuccinimide in DMF with ice cooling, the mixt. stirred 10 h with ice cooling, a mixt. of 1.2 g ampicillin-3H₂O and 0.42 mL Et_3N in CH_2CI_2 -DMF added, and the mixt. stirred 3 h at room temp. to give, after treating with K 2-ethylhexanoate, 1.32 d-I (R = 4-carbamoyl-2-quinolyl) K salt.

IT ***75204~90-9P***

> RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and bactericidal activity of)

RN 75204-90-9 CA

4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, CN

6-[[[[2-(aminocarbonyl)-4-quinolinyl]carbonyl]amino] phenylacetyl] amino] -3, 3-dimethyl-7-oxo-, aminocarbonyl] -4-quinolinyl] -4-quinolinmonopotassium salt, [2S-[2 α ,5 α ,6 β (S*)]]- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 147

L6 ANSWER 12 OF 17 CA COPYRIGHT 1997 ACS

DUPLICATE 12

AN 90:38949 CA

TI Cephalosporins with α -acylaminoacetic acid side chains

IN Kocsis, Karoly; Peter, Heinrich; Bickel, Hans

PA Ciba-Geigy A.-G., Switz.

SO Swiss, 11 pp.

CODEN: SWXXAS

PI CH 606006 781013

AI CH 74-6494 740513

DT Patent

LA German

GI

The cephalosporins I [R = 6-membered ring contg. 1-3 N atoms and an oxo group (optionally substituted or condensed with other rings); R1 = (substituted) Ph, thienyl, furyl, cyclohexadienyl; R2 = H, ester group; R3 = H, alkoxy, substituted Me] were prepd. for use as bactericides, e.g., at 8-100 mg/kg s.c. in mice against Staphylococcus aureus. Thus, D-(-)-(1,6-dihydro-6-oxo-3-pyridazinylcarbonylamino)phenylacetic acid reacted with ClCO₂Et, N-methylmorpholine, and 7β -aminocephalosporanic acid in THF to give D- 7β -I (R = 1,6-dihydro-6-oxo-3-pyridazinyl, R1 = Ph, R2 = H, R3 = AcOCH₂).

IT ***59133-55-0P***

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 59133-55-0 CA

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

 $3-[(acetyloxy)methyl]-7-[[[[(1,2-dihydro-2-oxo-4-quinolinyl)carbonyl]amino]phenylacetyl]amino]-8-oxo-, [6R-[6<math>\alpha$,7 β (R*)]]- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C 08 OCT 1997 20:02:57

PAGE 148

RN 59133-55-0 CA

Copyright © 1997 American Chemical Society (ACS)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 149

L6 ANSWER 13 OF 17 CA COPYRIGHT 1997 ACS

DUPLICATE 13

AN 90:38951 CA

TI Cephalosporins with α -acylaminoacetic acid side chains

IN Kocsis, Karoly; Peter, Heinrich; Bickel, Hans

PA Ciba-Geigy A.-G., Switz.

SO Swiss, 11 pp.

CODEN: SWXXAS

PI CH 606001 781013

AI CH 74-6494 740513

DT Patent

LA German

GI

AB The cephemcarboxylic acids I [R = 6-membered ring contg. 1-3 N atoms and an oxo group, optionally substituted or condensed with other rings; R^1 = (substituted) Ph, thienyl, furyl, cyclohexadienyl; R^2 = H, physiol. cleavable ester group; R^3 = H, (substituted) Me, lower alkoxy] were prepd. for use as bactericides, e.g., at 8-100 mg/kg s.c. against Staphylococcus aureus in mice. Thus, cephaloglycin reacted with 6-hydroxy-3-pyridinecarbonyl chloride in CH_2Cl_2 to give I (R = 6-hydroxy-3-pyridyl, R^1 = Ph, R^2 = H, R^3 = CH_2OAc).

IT ***59133-55-0P***

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 59133-55-0 CA

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[[[(1,2-dihydro-2-oxo-4-quinolinyl)carbonyl]amino]phenylacetyl]amino]-8-oxo-, [6R-[6 α ,7 β (R*)]]- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 151

L6 ANSWER 14 OF 17 CA COPYRIGHT 1997 ACS

DUPLICATE 14

AN 84:135637 CA

TI Penicillins

IN Tobiki, Hisao; Shimaji, Kozo; Okano, Shigeru; Komatsu, Toshiaki; Katsura, Toyozo; Taira, Yasushi: Eda, Yasuko

PA Sumitomo Chemical Co., Ltd., Japan

SO Japan., 11 pp.

CODEN: JAXXAD

PI JP 50023036 B4 750805 Showa

AI JP 70-124363 701229

DT Patent

LA Japanese

GI For diagram(s), see printed CA Issue.

Acids ROH I (Z = 0, S; R1 = alkyl, cycloalkylalkyl, alkenyl, aralkyl, OH, alkoxy, aralkyloxy; R2 = H, alkyl; A = benzo, naphtho, pyrido) were treated with 6-aminopenicillanic acid (III) or its derivs. to give II. II are bactericides not only against gram-pos. and -neg. bacteria but also against Pseudomonas aeruginosa (min. inhibitory concn. 3.13-50 .mu.g/ml). Thus, 2 g 1-hydroxy-6,7-methylenedioxy-4-quinolone-3-carboxylic acid in CH2Cl2 was treated with Et3N, 1.8 g CICO2Et, and 1.65 g D(-)-.alpha.-phenylglycine Et ester-HCl to give 1.8 g D(-)-.alpha.-(1-hydroxy-6,7-methylenedioxy-4-quinolone-3-carboxamido)phenylacetic acid, which (1 g) in CH2Cl2 was treated with Et3N, CICO2Et and 0.83 g III Et3N salt to give 1.3 g D(-)-II (Z = 0, R1 = OH, R2 = H, A = 6,7-methylenedioxybenzo). Among 25 more II prepd. were (Z, R1, R2, A given): 0, Et, H, 6-methoxybenzo; 0, Me, H, X; 0, Et, H, 1,2-naphtho; 0, OEt, H, 6,7-methylenedioxybenzo.

IT ***58865-82-0P***

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and bactericidal activity of)

RN 58865-82-0 CA

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, $6-[[[(3-ethoxy-4-quinolinyl)carbonyl]amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-, monosodium salt, \\ [2S-(2\alpha,5\alpha,6\beta)]- (9CI) (CA INDEX NAME)$

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 153

L6 ANSWER 15 OF 17 CA COPYRIGHT 1997 ACS

DUPLICATE 15

AN 84:164802 CA

TI Cephalosporins with .alpha.-acylaminoacetic acid side chain

IN Kocsis, Karoly; Peter, Heinrich; Bickel, Hans

PA Ciba-Geigy A.-G., Switz.

SO Ger. Offen., 80 pp.

CODEN: GWXXBX

PI DE 2520561 751127

PRAI CH 74-6494 740513

DT Patent

LA German

GI

AB Of the cephalosporins I (R = N heterocyclyl, R1 = CH2OAc, OMe, heterocyclic thiomethyl pyridiniomethyl) were prepd. by acetylating cephaloglycines and substituting on acetoxymethyl group. Thus, I (R = 2-hydroxy-5-pyridyl, R1 = OAc) was obtained by treating cephaloglycine with 2-hydroxy-5-pyridinecarbonyl chloride.

IT ***59133-55-0P***

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 59133-55-0 CA

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[(acetyloxy)methyl]-7-[[[[(1,2-dihydro-2-oxo-4-quinolinyl)carbonyl]amino]phenylacetyl]amino]-8-oxo-, [6R-[6 α ,7 β (R*)]]- (9CI) (CA INDEX NAME)

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 154

RN 59133-55-0 CA

L6 ANSWER 16 OF 17 CA COPYRIGHT 1997 ACS

DUPLICATE 16

AN 70:47439 CA

TI .alpha.-Amidobenzyl- and amido(2-thienyl)methylpenicillins

IN Long, Anthony Alfred W.; Nayler, John H. C.

PA Beecham Group Ltd.

SO Brit., 6 pp.

CODEN: BRXXAA

PI GB 1130445 681016

AI GB 660426

DT Patent

LA English

GI For diagram(s), see printed CA Issue.

AB The 6-aminopenicillanic acid derivs. prepd. had the structure I, where R is a Ph or thienyl group, R1 is a heterocyclic group, and n is 0 or 1. The compds. were useful as antibacterial agents, as nutritional supplements in animal food, and in the treatment of infectious diseases caused by gram-pos. and gram-neg. bacteria. Thus, a suspension of 12.8 g. D-.alpha.-aminobenzylpenicillin (II) trihydrate in 80 ml. H2O was adjusted to pH 9.2 with 5N aq. NaOH and treated with a soln. of 4.6 g. 5-methyl-3-isoxazolecarbonyl chloride in 100 ml. iso-BuCOMe (III). After stirring for 2 hrs. at room temp., the mixt. was filtered through Dicalite and the layers were sepd. The org. phase was washed with satd. brine and treated with 16 ml. 2N Na 2-ethylhexanoate in III to give 13 g. Na salt of

D-.alpha.-(5-methyl-3-iso-xazolecarboxamido)benzylpenicillin which crystd. on trituration with ether.

The sodium salts of D-.alpha.-(5-methyl-4-isoxazolecar-boxamido)benzylpenicillin,

D-.alpha.-(2-furancarboxamido)benzylpenicillin, D-.alpha.-(3-thiophenecarboxamido)benzylpenicillin,

D-.alpha.-(2-thiophenecarboxamido)benzylpenicillin, D-.alpha.-(2-thiopheneacetamido)benzylpenicillin,

D-.alpha.-(3-thiopheneacetamido)benzylpenicillin,

D-.alpha.-(3-ethoxy-4-quinolinecarboxamido)benzylpenicillin,

D-.alpha.-(8-methoxy-2-quinolinecarboxamido)benzylpenicillin,

D-.alpha.-(2-pyridinecarboxamido)benzylpenicillin, D-.alpha.-(phthalimidoacetamido)-benzylpenicillin,

D-.alpha.-(2,6-dioxo-4-piperidineacitamido)benzylpenicillin,

D-.alpha.-(2-oxo-2H-pyran-5-carboxamido)benzylpenicillin,

D-.alpha.-(5-methyl-3-phenyl-4-isoxazolecarboxamido)benzylpenicillin.

D-.alpha.-(3-methyl-5-phenyl-4-isoxazolecarboxamido)benzylpenicillin,

D-.alpha.-(5-bromo-2-(methylthio)-4-pyrimidinecarboxamido)benzylpenicillin,

D-.alpha.-(2-furoylamino)-2-thienylmethylpenicillin, D-.alpha.-nicotinamidobenzylpenicillin,

D-.alpha.-(2-thiopheneacetamido)-2-thi-enylmethylpenicillin, and

D-.alpha.-(2-furanacetamido)benzylpenicillin were similarly prepd.

IT ***21611-82-5P***

CA FILE SEARCH RESULTS - P281364C

08 OCT 1997 20:02:57

PAGE 156

CA COPYRIGHT 1997 ACS L6 ANSWER 17 OF 17

DUPLICATE 17

AN 74:87972

TI Antibacterial acylated benzylpenicillin and thienylmethylpenicillin derivatives

PA Beecham Group Ltd.

SO Fr. M., 4 pp.

CODEN: FMXXAJ

PΙ FR 6212 680902

PRAI GB 660426

DT **Patent**

LA French

GI For diagram(s), see printed CA Issue.

AB [.alpha.-(Amino)arylacetamido]penicillin deriv. (I), where Ar is Ph or 2-thienyl, are treated with Ar1(CH2)nCOCI (Ar1 = heteroaryl) to give penicillin diamide derivs. (II). II (n = 0 or 1 and Ar1 is furyl, thienyl, phthalimido, or a substituted quinolyl, piperidyl, oxopyranyl, or isoxazolyl group) are prepd.

IT ***21611-82-5P***

> RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

21611-82-5 CA

RN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, CN

> 6-[2-(3-ethoxycinchoninamido)-2-phenylacetamido]-3,3-dimethyl-7-oxo-, p- (8CI) (CA INDEX NAME)

Absolute stereochemistry.

Copyright © 1997 American Chemical Society (ACS)